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United States
Environmental Protection
Agency

Assessment of the Potential Impacts of Hydraulic Fracturing for Oil and Gas on Drinking Water Resources

Appendices A-J

Office of Research and Development
Washington, D.C.

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(Appendices A – J)

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Office of Research and Development
U.S. Environmental Protection Agency
Washington, DC 20460

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Appendix A

Chemicals Identified in Hydraulic Fracturing Fluids and/or Flowback and Produced Water

Appendix A. Chemicals Identified in Hydraulic Fracturing Fluids and/or Flowback and Produced Water

A.1. Supplemental Tables and Information

The EPA identified authoritative sources for information on hydraulic fracturing chemicals and, to the extent possible, verified the chemicals used in hydraulic fracturing fluids and detected in flowback and produced water of hydraulically fractured wells. The EPA used 10 sources to identify the chemicals used in hydraulic fracturing fluids or detected in flowback or produced water. Seven sources are government entities (Congressional, federal, or state) that obtained the data directly from industry. The remaining three represent collaborations between state, non-profit, academic, and industry groups. FracFocus is the result of a collaboration between the Ground Water Protection Council (a non-profit coalition of state ground water protection agencies) and the Interstate Oil and Gas Compact Commission (a multi-state government agency). The Marcellus Shale Coalition is a drilling industry trade group. Colborn et al. (2011) is a peer-reviewed journal article. Most of the listed chemicals were cited by multiple sources.

Seven of the ten sources obtained information about the chemicals used in hydraulic fracturing fluids from material safety data sheets (MSDSs) provided by chemical manufacturers for the products they sell, as required by the Occupational Safety and Health Administration (OSHA). The MSDSs must list all hazardous ingredients if they comprise at least 1% of the product; for carcinogens, the reporting threshold is 0.1%. However, chemical manufacturers may withhold information (e.g., chemical name, concentration of the substance in a mixture) about a hazardous substance from MSDSs if it is claimed as confidential business information (CBI), provided that certain conditions are met (OSHA, 2013).

Table A-1. Description of sources used to create lists of chemicals used in fracturing fluids or detected in flowback or produced water.

The number next to each citation in the reference column corresponds to numbers in the reference columns found in Table A-2, Table A-3, and Table A-4.

Description / Content	Reference
Chemicals and other components used by 14 hydraulic fracturing service companies from 2005 to 2009 as reported to the House Committee on Energy and Commerce. For each hydraulic fracturing product reported, companies also provided an MSDS with information about the product's chemical components.	House of Representatives (2011)[a] (1)

Description / Content	Reference
Chemicals used during natural gas operations with some potential health effects. The list of chemicals was compiled from MSDSs from several sources, including the Bureau of Land Management, U.S. Forest Service, state agencies, and industry.	Colborn et al. (2011)[a] (2)
Chemicals used or proposed for use in hydraulic fracturing in the Marcellus Shale in New York based on product composition disclosures and MSDSs submitted to the New York State Department of Environmental Conservation (NYSDEC). Also includes data provided separately to NYSDEC by well operators on analytical results of flowback water samples from Marcellus Shale operations in Pennsylvania and West Virginia.	NYSDEC (2011)[a,b] (3)
Chemicals reported to be used by nine hydraulic fracturing service companies from 2005 to 2010. Companies provided the chemical names in MSDSs, product bulletins, and formulation sheets.	U.S. EPA (2013a)[a] (4)
MSDSs provided to the EPA during on-site visits to hydraulically fractured oil and gas wells in Oklahoma and Colorado.	Sheets
Characteristics of undiluted chemicals found in hydraulic fracturing fluids associated with coalbed methane production, based on MSDSs, literature searches, reviews of relevant MSDSs provided by service companies, and discussions with field engineers, service company chemists, and state and federal employees.	U.S. EPA (2004)[a] (6)
Chemicals used in Pennsylvania for hydraulic fracturing activities based on MSDSs provided by industry.	PA DEP (2010)[a] (7)
Chemical records entered in FracFocus by oil and gas operators for individual wells from January 1, 2011, through February 28, 2013. FracFocus is a publicly accessible hydraulic fracturing chemical registry developed by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission. Chemicals claimed as confidential business information (CBI) do not have to be reported in FracFocus.	U.S. EPA (2015c)[a] (8)
Chemicals detected in flowback from 19 hydraulically fractured shale gas wells in Pennsylvania and West Virginia, based on analyses conducted by 17 Marcellus Shale Coalition member companies.	Hayes (2009)[b] (9)
Chemicals reportedly detected in flowback and produced water from 81 wells provided to the EPA by nine well operating companies.	U.S. EPA (2011b)[b] (10)

[a] Sources used to identify chemicals used in hydraulic fracturing fluids.

[b] Sources used to identify chemicals detected in flowback and produced water.

Once it had identified chemicals used in hydraulic fracturing fluids and chemicals detected in flowback/produced water, the EPA conducted an initial review of the chemicals for preliminary validation of provided chemical name and Chemical Abstracts Service Registry Number (CASRN) combinations. A CASRN is a unique numeric identifier assigned by the Chemical Abstracts Service (CAS) to a chemical substance when it enters the CAS Registry Database. The EPA Office of Research

and Development's National Center for Computational Toxicology (NCCT) provided the final formal validation and verification of the listed chemicals.

The EPA first compared the hydraulic fracturing chemical CASRNs and names with chemicals listed in NCCT's Distributed Structure-Searchable Toxicity Database network (DSSTox) database (U.S. EPA, 2013b). For the CASRNs and chemical names that did not appear in the DSSTox database, the EPA's Substance Registry Services database and the U.S. National Library of Medicine ChemID database were used to verify accurate chemical name and CASRN pairing (NLM, 2014; U.S. EPA, 2014c). The EPA also identified cases where CASRN/name combinations could not be verified by use of selected public sources and flagged those cases for resolution by NCCT.

NCCT then verified all of the CASRN and chemical names for the chemical lists generated by the EPA in accordance with NCCT DSSTox Chemical Information Quality Review Procedures (http://www.epa.gov/ncct/dsstox/ChemicalInfQAProcedures.html). The process included QA/QC on the identification and validation of CASRN/chemical name combinations and resolution of inconsistencies and problems including duplications, CASRN errors, and CASRN/chemical name mismatches.

The general methodology for resolving conflicts between CASRN/chemical name combinations and other chemical identification issues differed slightly depending on the data provided by each source. To resolve chemical/CASRN conflict in data provided by the nine service companies, the EPA worked with each company to verify the CASRN/chemical combinations proposed by NCCT. In cases of CASRN/chemical name mismatches in data provided by FracFocus, chemical names were considered primary to the CASRN (i.e., the name overrode the CASRN). When the chemical name was non-specific and the CASRN was valid, then the CASRN was considered primary to the chemical name, and the correct specific chemical name from DSSTox was assigned to the CASRN. For all other sources, the CASRN was considered primary unless it was invalid or missing. In such cases, the chemical name was primary. All Toxic Substance Control Act (TSCA) CBI chemical lists were managed in accordance with TSCA CBI procedures.

Chemicals with verified CASRNs that are used in hydraulic fracturing fluids are presented in Table A-2. Generic chemicals used in hydraulic fracturing fluids are presented in Table A-3. Chemicals with verified CASRNs that have been detected in flowback or produced water are presented in Table A-4. Chemicals found in both fracturing fluids (see Table A-2) and flowback and produced water (see Table A-4) are italicized in each table.

Table A-2. Chemicals reported to be used in hydraulic fracturing fluids.

An "X" indicates the availability of physicochemical properties from EPI Suite™ (see Appendix C) and selected toxicity reference values (see Appendix G). An empty cell indicates no information was available from the sources we consulted. Reference number corresponds to the citations in Table A-1. Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
(13Z)-N,N-bis(2-hydroxyethyl)-N-methyldocos-13-en-1-aminium chloride	120086-58-0	X		1
(2,3-dihydroxypropyl)trimethylammonium chloride	34004-36-9	X		8
(E)-Crotonaldehyde	123-73-9	X	X	1, 4
[Nitrilotris(methylene)]tris-phosphonic acid pentasodium salt	2235-43-0	X		1
1-(1-Naphthylmethyl)quinolinium chloride	65322-65-8	X		1
1-(Alkyl* amino)-3-aminopropane *(42%C12, 26%C18, 15%C14, 8%C16, 5%C10, 4%C8)	68155-37-3	X		8
1-(Phenylmethyl)pyridinium Et Me derivs., chlorides	68909-18-2	X		1, 2, 3, 4, 6, 8
1,2,3-Trimethylbenzene	526-73-8	X		1, 4
1,2,4-Trimethylbenzene	*95-63-6*	X		*1, 2, 3, 4, 5*
1,2-Benzisothiazolin-3-one	2634-33-5	X		1, 3, 4
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	X		1, 4
1,2-Dimethylbenzene	95-47-6	X		4
1,2-Ethanediamine, polymer with 2-methyloxirane	25214-63-5			8
1,2-Ethanediaminium, N,N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4	X		1, 4
1,2-Propylene glycol	*57-55-6*	X	X	*1, 2, 3, 4, 8*
1,2-Propylene oxide	75-56-9	X	X	1, 4
1,3,5-Triazine	290-87-9	X		8
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	X		1, 4
1,3,5-Trimethylbenzene	*108-67-8*	X		*1, 4*
1,3-Butadiene	106-99-0	X	X	8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1,3-Dichloropropene	542-75-6	X	X	8
1,4-Dioxane	123-91-1	X	X	2, 3, 4
1,4-Dioxane-2,5-dione, 3,6-dimethyl-, (3R,6R)-, polymer with (3S,6S)-3,6-dimethyl-1,4-dioxane-2,5-dione and (3R,6S)-rel-3,6-dimethyl-1,4-dioxane-2,5-dione	9051-89-2			1, 4, 8
1,6-Hexanediamine	124-09-4	X		1, 2
1,6-Hexanediamine dihydrochloride	6055-52-3	X		1
1-[2-(2-Methoxy-1-methylethoxy)-1-methylethoxy]-2-propanol	20324-33-8	X		4
1-Amino-2-propanol	78-96-6	X		8
1-Benzylquinolinium chloride	15619-48-4	X		1, 3, 4
1-Butanol	71-36-3	X	X	1, 2, 3, 4, 7
1-Butoxy-2-propanol	5131-66-8	X		8
1-Decanol	112-30-1	X		1, 4
1-Dodecyl-2-pyrrolidinone	2687-96-9	X		1, 4
1-Eicosene	3452-07-1	X		3
1-Ethyl-2-methylbenzene	611-14-3	X		4
1-Hexadecene	629-73-2	X		3
1-Hexanol	111-27-3	X		1, 4, 8
1-Hexanol, 2-ethyl-, manuf. of, by products from, distn. residues	68909-68-7			4
1H-Imidazole-1-ethanamine, 4,5-dihydro-, 2-nortall-oil alkyl derivs.	68442-97-7			2, 4
1-Methoxy-2-propanol	107-98-2	X		1, 2, 3, 4
1-Octadecanamine, acetate (1:1)	2190-04-7	X		8
1-Octadecanamine, N,N-dimethyl-	124-28-7	X		1, 3, 4
1-Octadecene	112-88-9	X		3
1-Octanol	111-87-5	X		1, 4
1-Pentanol	71-41-0	X		8
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., chlorides, sodium salts	61789-39-7			1

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., inner salts	61789-40-0			1, 2, 3, 4
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3327-22-8	X		8
1-Propanaminium, N-(3-aminopropyl)-2-hydroxy-N,N-dimethyl-3-sulfo-, N-coco acyl derivs., inner salts	68139-30-0			1, 3, 4
1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[(1-oxooctyl)amino]-, inner salt	73772-46-0			8
1-Propanesulfonic acid	5284-66-2	X		3
1-Propanol	71-23-8	X		1, 2, 4, 5
1-Propanol, zirconium(4+) salt	23519-77-9			1, 4, 8
1-Propene	115-07-1	X		2
1-tert-Butoxy-2-propanol	57018-52-7	X		8
1-Tetradecene	1120-36-1	X		3
1-Tridecanol	112-70-9	X		1, 4
1-Undecanol	112-42-5	X		2
2-(2-Butoxyethoxy)ethanol	112-34-5	X	X	2, 4
2-(2-Ethoxyethoxy)ethanol	111-90-0	X	X	1, 4
2-(2-Ethoxyethoxy)ethyl acetate	112-15-2	X		1, 4
2-(Dibutylamino)ethanol	102-81-8	X		1, 4
2-(Hydroxymethylamino)ethanol	34375-28-5	X		1, 4
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	X	X	2
2,2'-(diazene-1,2-diyldiethane-1,1-diyl)bis-4,5-dihydro-1H-imidazole dihydrochloride	27776-21-2	X		3
2,2'-(Octadecylimino)diethanol	10213-78-2	X		1
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	X		1, 4
2,2'-Azobis(2-amidinopropane) dihydrochloride	2997-92-4	X		1, 4
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	X		1, 2, 3, 4, 6, 7, 8
2,2-Dibromopropanediamide	73003-80-2	X		3
2,4-Hexadienoic acid, potassium salt, (2E,4E)-	24634-61-5	X		3

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2,6,8-Trimethyl-4-nonanol	123-17-1	X		8
2-Acrylamide - 2-propanesulfonic acid and N,N-dimethylacrylamide copolymer	NOCAS_51252			2
2-Acrylamido -2-methylpropanesulfonic acid copolymer	NOCAS_51255			8
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	X		1, 3
2-Amino-2-methylpropan-1-ol	124-68-5	X		8
2-Aminoethanol ester with boric acid (H3BO3) (1:1)	10377-81-8			8
2-Aminoethanol hydrochloride	2002-24-6	X		4, 8
2-Bromo-3-nitrilopropionamide	1113-55-9	X		1, 2, 3, 4, 5
2-Butanone oxime	96-29-7	X		1
2-Butenediamide, (2E)-, N,N'-bis[2-(4,5-dihydro-2-nortall-oil alkyl-1H-imidazol-1-yl)ethyl] derivs.	68442-77-3			3, 8
2-Butoxy-1-propanol	15821-83-7	X		8
2-Butoxyethanol	111-76-2	X	X	1, 2, 3, 4, 6, 7, 8
2-Dodecylbenzenesulfonic acid- n-(2-aminoethyl)ethane-1,2-diamine(1:1)	40139-72-8	X		8
2-Ethoxyethanol	110-80-5	X	X	6
2-Ethoxynaphthalene	93-18-5	X		3
2-Ethyl-1-hexanol	104-76-7	X		1, 2, 3, 4, 5
2-Ethyl-2-hexenal	645-62-5	X		2
2-Ethylhexyl benzoate	5444-75-7	X		4
2-Hydroxyethyl acrylate	818-61-1	X		1, 4
2-Hydroxyethylammonium hydrogen sulphite	13427-63-9	X		1
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	7006-59-9	X		8
2-Mercaptoethanol	60-24-2	X		1, 4
2-Methoxyethanol	109-86-4	X	X	4
2-Methyl-1-propanol	78-83-1	X	X	1, 2, 4
2-Methyl-2,4-pentanediol	107-41-5	X		1, 2, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2-Methyl-3(2H)-isothiazolone	2682-20-4	X		1, 2, 4
2-Methyl-3-butyn-2-ol	115-19-5	X		3
2-Methylbutane	78-78-4	X		2
2-Methylquinoline hydrochloride	62763-89-7	X		3
2-Phosphono-1,2,4-butanetricarboxylic acid	37971-36-1	X		1, 4
2-Phosphonobutane-1,2,4-tricarboxylic acid, potassium salt (1:x)	93858-78-7	X		1
2-Propanol, aluminum salt	555-31-7			1
2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	26062-79-3			3
2-Propenamide, homopolymer	25038-45-3			8
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	13533-05-6	X		4
2-Propenoic acid, 2-ethylhexyl ester, polymer with 2-hydroxyethyl 2-propenoate	36089-45-9			8
2-Propenoic acid, 2-methyl-, polymer with 2-propenoic acid, sodium salt	28205-96-1			8
2-Propenoic acid, 2-methyl-, polymer with sodium 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonate (1:1)	136793-29-8			8
2-Propenoic acid, ethyl ester, polymer with ethenyl acetate and 2,5-furandione, hydrolyzed	113221-69-5			4, 8
2-Propenoic acid, ethyl ester, polymer with ethenyl acetate and 2,5-furandione, hydrolyzed, sodium salt	111560-38-4			8
2-Propenoic acid, polymer with 2-propenamide, sodium salt	25987-30-8			3, 4, 8
2-Propenoic acid, polymer with ethene, zinc salt	28208-80-2			8
2-Propenoic acid, polymer with ethenylbenzene	25085-34-1			8
2-Propenoic acid, polymer with sodium ethanesulfonate, peroxydisulfuric acid, disodium salt- initiated, reaction products with tetrasodium ethenylidenebis (phosphonata)	397256-50-7			8
2-Propenoic acid, polymer with sodium phosphinate (1:1), sodium salt	129898-01-7			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2-Propenoic acid, sodium salt (1:1), polymer with sodium 2-methyl-2-((1-oxo-2-propen-1-yl)amino)-1-propanesulfonate (1:1)	37350-42-8			1
2-Propenoic acid, telomer with sodium 4-ethenylbenzenesulfonate (1:1), sodium 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonate (1:1) and sodium sulfite (1:1), sodium salt	151006-66-5			4
2-Propenoic, polymer with sodium phosphinate	71050-62-9			3, 4
3-(Dimethylamino)propylamine	109-55-7	**X**		8
3,4,4-Trimethyloxazolidine	75673-43-7	**X**		8
3,5,7-Triazatricyclo(3.3.1.13,7)decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-	51229-78-8	**X**		3
3,7-Dimethyl-2,6-octadienal	5392-40-5	**X**		3
3-Hydroxybutanal	107-89-1	**X**		1, 2, 4
3-Methoxypropylamine	5332-73-0	**X**		8
3-Phenylprop-2-enal	104-55-2	**X**		1, 2, 3, 4, 7
4,4-Dimethyloxazolidine	51200-87-4	**X**		8
4,6-Dimethyl-2-heptanone	19549-80-5	**X**		8
4-[Abieta-8,11,13-trien-18-yl(3-oxo-3-phenylpropyl)amino]butan-2-one hydrochloride	143106-84-7	**X**		1, 4
4-Ethyloct-1-yn-3-ol	5877-42-9	**X**		1, 2, 3, 4
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	**X**		3
4-Methoxybenzyl formate	122-91-8	**X**		3
4-Methoxyphenol	150-76-5	**X**		4
4-Methyl-2-pentanol	108-11-2	**X**		1, 4
4-Methyl-2-pentanone	108-10-1	**X**		5
4-Nonylphenol	104-40-5	**X**		8
4-Nonylphenol polyethoxylate	68412-54-4			2, 3, 4
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	**X**		1, 2, 4
Acetaldehyde	75-07-0	**X**		1, 4
Acetic acid	*64-19-7*	**X**		*1, 2, 3, 4, 5, 6, 7, 8*

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Acetic acid ethenyl ester, polymer with ethenol	25213-24-5			1, 4
Acetic acid, C6-8-branched alkyl esters	90438-79-2	**X**		4
Acetic acid, hydroxy-, reaction products with triethanolamine	68442-62-6	**X**		3
Acetic acid, mercapto-, monoammonium salt	5421-46-5	**X**		2, 8
Acetic anhydride	108-24-7	**X**		1, 2, 3, 4, 7
Acetone	*67-64-1*	**X**	**X**	*1, 3, 4, 6*
Acetonitrile, 2,2',2''-nitrilotris-	7327-60-8	**X**		1, 4
Acetophenone	*98-86-2*	**X**	**X**	*1*
Acetyltriethyl citrate	77-89-4	**X**		1, 4
Acrolein	*107-02-8*	**X**	**X**	*2*
Acrylamide	79-06-1	**X**	**X**	1, 2, 3, 4
Acrylamide/ sodium acrylate copolymer	25085-02-3			1, 2, 3, 4, 8
Acrylamide-sodium-2-acrylamido-2-methlypropane sulfonate copolymer	38193-60-1			1, 2, 3, 4
Acrylic acid	79-10-7	**X**	**X**	2, 4
Acrylic acid, with sodium-2-acrylamido-2-methyl-1-propanesulfonate and sodium phosphinate	110224-99-2	**X**		8
Alcohols (C13-C15), ethoxylated	64425-86-1			8
Alcohols, C10-12, ethoxylated	67254-71-1	**X**		3
Alcohols, C10-14, ethoxylated	66455-15-0			3
Alcohols, C11-14-iso-, C13-rich	68526-86-3	**X**		3
Alcohols, C11-14-iso-, C13-rich, butoxylated ethoxylated	228414-35-5			1
Alcohols, C11-14-iso-, C13-rich, ethoxylated	78330-21-9	**X**		3, 4, 8
Alcohols, C12-13, ethoxylated	66455-14-9	**X**		4
Alcohols, C12-14, ethoxylated	68439-50-9			2, 3, 4, 8
Alcohols, C12-14, ethoxylated propoxylated	68439-51-0	**X**		1, 3, 4, 8
Alcohols, C12-14-secondary	126950-60-5	**X**		1, 3, 4
Alcohols, C12-14-secondary, ethoxylated	84133-50-6			3, 4, 8
Alcohols, C12-15, ethoxylated	68131-39-5			3, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Alcohols, C12-16, ethoxylated	68551-12-2	**X**		3, 4, 8
Alcohols, C14-15, ethoxylated	68951-67-7	**X**		3, 4, 8
Alcohols, C6-12, ethoxylated	68439-45-2	**X**		3, 4, 8
Alcohols, C7-9-iso-, C8-rich, ethoxylated	78330-19-5	**X**		2, 4, 8
Alcohols, C8-10, ethoxylated propoxylated	68603-25-8			3
Alcohols, C9-11, ethoxylated	68439-46-3	**X**		3, 4
Alcohols, C9-11-iso-, C10-rich, ethoxylated	78330-20-8	**X**		1, 2, 4, 8
Alkanes C10-16-branched and linear	90622-52-9			4
Alkanes, C10-14	93924-07-3			1
Alkanes, C12-14-iso-	68551-19-9	**X**		2, 4, 8
Alkanes, C13-16-iso-	68551-20-2	**X**		1, 4
Alkenes, C>10 .alpha.-	64743-02-8	**X**		1, 3, 4, 8
Alkenes, C>8	68411-00-7			1
Alkenes, C24-25 alpha-, polymers with maleic anhydride, docosyl esters	68607-07-8			8
Alkyl quaternary ammonium with bentonite	71011-24-0			4
Alkyl* dimethyl ethylbenzyl ammonium chloride *(50%C12, 30%C14, 17%C16, 3%C18)	85409-23-0_1	**X**		8
Alkyl* dimethyl ethylbenzyl ammonium chloride *(60%C14, 30%C16, 5%C12, 5%C18)	68956-79-6	**X**		8
Alkylbenzenesulfonate, linear	42615-29-2	**X**		1, 4, 6
Almandite and pyrope garnet	1302-62-1			1, 4
alpha-[3.5-dimethyl-1-(2-methylpropyl)hexyl]-omega-hydroxy-poly(oxy-1,2-ethandiyl)	60828-78-6			3
alpha-Amylase	9000-90-2			4
alpha-Lactose monohydrate	5989-81-1	**X**		8
alpha-Terpineol	98-55-5	**X**		3
Alumina	1344-28-1			1, 2, 4
Aluminatesilicate	1327-36-2			8
Aluminum	*7429-90-5*		**X**	*1, 4, 6*
Aluminum calcium oxide (Al2CaO4)	12042-68-1			2

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Aluminum chloride	7446-70-0			1, 4
Aluminum chloride hydroxide sulfate	39290-78-3			8
Aluminum chloride, basic	1327-41-9			3, 4
Aluminum oxide (Al2O3)	90669-62-8			8
Aluminum oxide silicate	12068-56-3			1, 2, 4
Aluminum silicate	12141-46-7			1, 2, 4
Aluminum sulfate	10043-01-3			1, 4
Amaranth	915-67-3	**X**		4
Amides, C8-18 and C18-unsatd., N,N-bis(hydroxyethyl)	68155-07-7			3
Amides, coco, N-[3-(dimethylamino)propyl]	68140-01-2			1, 4
Amides, coco, N-[3-(dimethylamino)propyl], alkylation products with chloroacetic acid, sodium salts	70851-07-9			1, 4
Amides, coco, N-[3-(dimethylamino)propyl], alkylation products with sodium 3-chloro-2-hydroxypropanesulfonate	70851-08-0			8
Amides, coco, N-[3-(dimethylamino)propyl], N-oxides	68155-09-9			1, 3, 4
Amides, from C16-22 fatty acids and diethylenetriamine	68876-82-4			3
Amides, tall-oil fatty, N,N-bis(hydroxyethyl)	68155-20-4			3, 4
Amides, tallow, N-[3-(dimethylamino)propyl],N-oxides	68647-77-8			1, 4
Amine oxides, cocoalkyldimethyl	61788-90-7			8
Amines, C14-18; C16-18-unsaturated, alkyl, ethoxylated	68155-39-5			1
Amines, C8-18 and C18-unsatd. alkyl	68037-94-5			5
Amines, coco alkyl	61788-46-3			4
Amines, coco alkyl, acetates	61790-57-6			1, 4
Amines, coco alkyl, ethoxylated	61791-14-8			8
Amines, coco alkyldimethyl	61788-93-0			8
Amines, dicoco alkyl	61789-76-2			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Amines, dicoco alkylmethyl	61788-62-3			8
Amines, ditallow alkyl, acetates	71011-03-5			8
Amines, hydrogenated tallow alkyl, acetates	61790-59-8			4
Amines, N-tallow alkyltrimethylenedi-, ethoxylated	61790-85-0			8
Amines, polyethylenepoly-, ethoxylated, phosphonomethylated	68966-36-9			1, 4
Amines, polyethylenepoly-, reaction products with benzyl chloride	68603-67-8			1
Amines, tallow alkyl	61790-33-8			8
Amines, tallow alkyl, ethoxylated, acetates (salts)	68551-33-7			1, 3, 4
Amines, tallow alkyl, ethoxylated, phosphates	68308-48-5			4
Aminotrimethylene phosphonic acid	6419-19-8	**X**		1, 4, 8
Ammonia	*7664-41-7*			*1, 2, 3, 4, 7*
Ammonium (lauryloxypolyethoxy)ethyl sulfate	32612-48-9			4
Ammonium acetate	631-61-8	**X**		1, 3, 4, 5, 8
Ammonium acrylate	10604-69-0	**X**		8
Ammonium acrylate-acrylamide polymer	26100-47-0			2, 4, 8
Ammonium bisulfate	7803-63-6			2
Ammonium bisulfite	10192-30-0			1, 2, 3, 4, 7
Ammonium chloride	12125-02-9			1, 2, 3, 4, 5, 6, 8
Ammonium citrate (1:1)	7632-50-0	**X**		3
Ammonium citrate (2:1)	3012-65-5	**X**		8
Ammonium dodecyl sulfate	2235-54-3	**X**		1
Ammonium fluoride	12125-01-8			1, 4
Ammonium hydrogen carbonate	1066-33-7	**X**		1, 4
Ammonium hydrogen difluoride	1341-49-7			1, 3, 4, 7
Ammonium hydrogen phosphonate	13446-12-3			4
Ammonium hydroxide	1336-21-6			1, 3, 4
Ammonium lactate	515-98-0	**X**		8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Ammonium ligninsulfonate	8061-53-8			2
Ammonium nitrate	6484-52-2			1, 2, 3
Ammonium phosphate	7722-76-1		**X**	1, 4
Ammonium sulfate	7783-20-2			1, 2, 3, 4, 6
Ammonium thiosulfate	7783-18-8			8
Amorphous silica	99439-28-8			1, 7
Anethole	104-46-1	**X**		3
Aniline	62-53-3	**X**	**X**	2, 4
Antimony pentoxide	1314-60-9			1, 4
Antimony trichloride	10025-91-9		**X**	1, 4
Antimony trioxide	1309-64-4		**X**	8
Arsenic	*7440-38-2*		**X**	*4*
Ashes, residues	68131-74-8			4
Asphalt, sulfonated, sodium salt	68201-32-1			2
Attapulgite	12174-11-7			2, 3
Aziridine, polymer with 2-methyloxirane	31974-35-3			4, 8
Barium sulfate	7727-43-7			1, 2, 4
Bauxite	1318-16-7			1, 2, 4
Benactyzine hydrochloride	57-37-4	**X**		8
Bentonite	1302-78-9			1, 2, 4, 6
Bentonite, benzyl(hydrogenated tallow alkyl) dimethylammonium stearate complex	121888-68-4			3, 4
Benzamorf	12068-08-5	**X**		1, 4
Benzene	*71-43-2*	**X**	**X**	*1, 3, 4*
Benzene, 1,1'-oxybis-, sec-hexyl derivs., sulfonated, sodium salts	147732-60-3			8
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8			8
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated, sodium salts	119345-04-9			3, 4, 8
Benzene, C10-16-alkyl derivs.	68648-87-3	**X**		1

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Benzene, ethenyl-, polymer with 2-methyl-1,3-butadiene, hydrogenated	68648-89-5			8
Benzenemethanaminium, N,N-dimethyl-N-(2-((1-oxo-2-propen-1-yl)oxy)ethyl)-, chloride (1:1), polymer with 2-propenamide	74153-51-8			3
Benzenesulfonic acid	98-11-3	**X**		2
Benzenesulfonic acid, (1-methylethyl)-,	37953-05-2	**X**		4
Benzenesulfonic acid, (1-methylethyl)-, ammonium salt	37475-88-0	**X**		3, 4
Benzenesulfonic acid, (1-methylethyl)-, sodium salt	28348-53-0	**X**		8
Benzenesulfonic acid, C10-16-alkyl derivs.	68584-22-5		**X**	1, 4
Benzenesulfonic acid, C10-16-alkyl derivs., compds. with cyclohexylamine	255043-08-4	**X**		1
Benzenesulfonic acid, C10-16-alkyl derivs., compds. with triethanolamine	68584-25-8	**X**		8
Benzenesulfonic acid, C10-16-alkyl derivs., potassium salts	68584-27-0	**X**		1, 4, 8
Benzenesulfonic acid, dodecyl-, branched, compds. with 2-propanamine	90218-35-2	**X**		4
Benzenesulfonic acid, mono-C10-16 alkyl derivs., compds. with 2-propanamine	68648-81-7			1, 4
Benzenesulfonic acid, mono-C10-16-alkyl derivs., sodium salts	68081-81-2	**X**		8
Benzoic acid	65-85-0	**X**	**X**	1, 4, 7
Benzyl chloride	100-44-7	**X**	**X**	1, 2, 4, 8
Benzyldimethyldodecylammonium chloride	139-07-1	**X**		2, 8
Benzylhexadecyldimethylammonium chloride	122-18-9	**X**		8
Benzyltrimethylammonium chloride	56-93-9	**X**		8
Bicine	150-25-4	**X**		1, 4
Bio-Perge	55965-84-9			8
Bis(1-methylethyl)naphthalenesulfonic acid, cyclohexylamine salt	68425-61-6	**X**		1
Bis(2-chloroethyl) ether	*111-44-4*	**X**	**X**	*8*

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Bisphenol A	80-05-7	X	X	4
Bisphenol A/ Epichlorohydrin resin	25068-38-6			1, 2, 4
Bisphenol A/ Novolac epoxy resin	28906-96-9			1, 4
Blast furnace slag	65996-69-2			2, 3
Borax	1303-96-4			1, 2, 3, 4, 6
Boric acid	10043-35-3			1, 2, 3, 4, 6, 7
Boric acid (H3BO3), compd. with 2-aminoethanol (1:x)	26038-87-9			8
Boric oxide	1303-86-2			1, 2, 3, 4
Boron potassium oxide (B4K2O7)	1332-77-0			8
Boron potassium oxide (B4K2O7), tetrahydrate	12045-78-2			8
Boron potassium oxide (B5KO8)	11128-29-3			1
Boron sodium oxide	1330-43-4			1, 2, 4
Boron sodium oxide pentahydrate	12179-04-3			8
Bronopol	52-51-7	X		1, 2, 3, 4, 6
Butane	106-97-8	X		2, 5
Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	2373-38-8	X		1
Butene	25167-67-3	X		8
Butyl glycidyl ether	2426-08-6	X		1, 4
Butyl lactate	138-22-7	X		1, 4
Butyryl trihexyl citrate	82469-79-2	X		8
C.I. Acid Red 1	3734-67-6	X		4
C.I. Acid violet 12, disodium salt	6625-46-3	X		4
C.I. Pigment Red 5	6410-41-9	X		4
C.I. Solvent Red 26	4477-79-6	X		4
C10-16-Alkyldimethylamines oxides	70592-80-2	X		4
C10-C16 ethoxylated alcohol	68002-97-1	X		1, 2, 3, 4, 8
C11-15-Secondary alcohols ethoxylated	68131-40-8			1, 2, 8
C12-14 tert-alkyl ethoxylated amines	73138-27-9	X		3
C8-10 Alcohols	85566-12-7			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Calcined bauxite	66402-68-4			2, 8
Calcium aluminate	12042-78-3			2
Calcium bromide	7789-41-5			4
Calcium carbide (CaC2)	75-20-7			8
Calcium chloride	10043-52-4			1, 2, 3, 4, 7
Calcium dichloride dihydrate	10035-04-8			1, 4
Calcium dodecylbenzene sulfonate	26264-06-2	X		4
Calcium fluoride	7789-75-5			1, 4
Calcium hydroxide	1305-62-0			1, 2, 3, 4
Calcium hypochlorite	7778-54-3			1, 2, 4
Calcium magnesium hydroxide oxide	58398-71-3			4
Calcium oxide	1305-78-8			1, 2, 4, 7
Calcium peroxide	1305-79-9			1, 3, 4, 8
Calcium sulfate	7778-18-9			1, 2, 4
Calcium sulfate dihydrate	10101-41-4			2
Camphor	76-22-2	X		3
Canola oil	120962-03-0			8
Carbon black	1333-86-4			1, 2, 4
Carbon dioxide	*124-38-9*	X		*1, 3, 4, 6*
Carbonic acid calcium salt (1:1)	471-34-1			1, 2, 4
Carbonic acid, dipotassium salt	584-08-7	X		1, 2, 3, 4, 8
Carboxymethyl guar gum, sodium salt	39346-76-4			1, 2, 4
Castor oil	8001-79-4			8
Cedarwood oil	8000-27-9			3
Cellophane	9005-81-6			1, 4
Cellulose	9004-34-6			1, 2, 3, 4
Chloride	*16887-00-6*			*4, 8*
Chlorine	*7782-50-5*		X	*2*
Chlorine dioxide	10049-04-4		X	1, 2, 3, 4, 8
Choline bicarbonate	78-73-9	X		3, 8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Choline chloride	67-48-1	X		1, 3, 4, 7, 8
Chromium (III)	*16065-83-1*		X	*2, 6*
Chromium (VI)	*18540-29-9*		X	*6*
Chromium acetate, basic	39430-51-8			2
Chromium(III) acetate	1066-30-4			1, 2
Citric acid	77-92-9	X		1, 2, 3, 4, 7
Citronella oil	8000-29-1			3
Citronellol	106-22-9	X		3
Citrus extract	94266-47-4			1, 3, 4, 8
Coal, granular	50815-10-6			1, 2, 4
Cobalt(II) acetate	71-48-7			1, 4
Coco-betaine	68424-94-2			3
Coconut oil	8001-31-8			8
Coconut oil acid/Diethanolamine condensate (2:1)	68603-42-9			1
Coconut trimethylammonium chloride	61789-18-2	X		1, 8
Copper	*7440-50-8*		X	*1, 4*
Copper sulfate	7758-98-7			1, 4, 8
Copper(I) chloride	7758-89-6			1, 4
Copper(I) iodide	7681-65-4		X	1, 2, 4, 6
Copper(II) chloride	7447-39-4			1, 3, 4
Copper(II) sulfate, pentahydrate	7758-99-8			8
Corn flour	68525-86-0			4
Corn sugar gum	11138-66-2			1, 2, 4
Corundum (Aluminum oxide)	1302-74-5			4, 8
Cottonseed, flour	68308-87-2			2, 4
Coumarin	91-64-5	X		3
Cremophor(R) EL	61791-12-6			1, 3
Cristobalite	14464-46-1			1, 2, 4
Crystalline silica, tridymite	15468-32-3			1, 2, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Cumene	*98-82-8*	**X**	**X**	*1, 2, 3, 4*
Cupric chloride dihydrate	10125-13-0			1, 4, 7
Cyclohexane	110-82-7	**X**		1, 7
Cyclohexanol	108-93-0	**X**		8
Cyclohexanone	108-94-1	**X**	**X**	1, 4
Cyclohexylamine sulfate	19834-02-7	**X**		8
D&C Red 28	18472-87-2	**X**		4
D&C Red No. 33	3567-66-6	**X**		8
Daidzein	486-66-8	**X**		8
Dapsone	80-08-0	**X**		1, 4
Dazomet	533-74-4	**X**		1, 2, 3, 4, 7, 8
Decamethylcyclopentasiloxane	541-02-6			8
Decyldimethylamine	1120-24-7	**X**		3, 4
Deuterium oxide	7789-20-0			8
D-Glucitol	50-70-4	**X**		1, 3, 4
D-Gluconic acid	526-95-4	**X**		1, 4
D-Glucopyranoside, methyl	3149-68-6	**X**		2
D-Glucose	50-99-7	**X**		1, 4
Di(2-ethylhexyl) phthalate	*117-81-7*	**X**	**X**	*1, 4*
Diammonium peroxydisulfate	7727-54-0			1, 2, 3, 4, 6, 7, 8
Diatomaceous earth	68855-54-9			2, 4
Diatomaceous earth, calcined	91053-39-3			1, 2, 4
Dibromoacetonitrile	3252-43-5	**X**		1, 2, 3, 4, 8
Dicalcium silicate	10034-77-2			1, 2, 4
Dichloromethane	*75-09-2*	**X**	**X**	*8*
Didecyldimethylammonium chloride	7173-51-5	**X**	**X**	1, 2, 4, 8
Diethanolamine	111-42-2	**X**		1, 2, 3, 4, 6
Diethylbenzene	25340-17-4	**X**		1, 3, 4
Diethylene glycol	111-46-6	**X**		1, 2, 3, 4, 7

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Diethylene glycol monomethyl ether	111-77-3	X		1, 2, 4
Diethylenetriamine	111-40-0	X		1, 2, 4, 5
Diethylenetriamine reaction product with fatty acid dimers	68647-57-4			2
Diisobutyl ketone	108-83-8	X		8
Diisopropanolamine	110-97-4	X		8
Diisopropylnaphthalene	38640-62-9	X		3, 4
Dimethyl adipate	627-93-0	X		8
Dimethyl glutarate	1119-40-0	X		1, 4
Dimethyl polysiloxane	63148-62-9			1, 2, 4
Dimethyl succinate	106-65-0	X		8
Dimethylaminoethanol	108-01-0	X		2, 4
Dimethyldiallylammonium chloride	7398-69-8	X		3, 4
Diphenyl oxide	101-84-8	X		3
Dipotassium monohydrogen phosphate	7758-11-4			5
Dipropylene glycol	25265-71-8	X		1, 3, 4
Di-sec-butylphenol	31291-60-8	X		1
Disodium dodecyl(sulphonatophenoxy) benzenesulphonate	28519-02-0	X		1
Disodium ethylenediaminediacetate	38011-25-5	X		1, 4
Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	X		1
Disodium octaborate	12008-41-2			4, 8
Disodium octaborate tetrahydrate	12280-03-4			1, 4
Disodium sulfide	1313-82-2			8
Distillates, petroleum, catalytic reformer fractionator residue, low-boiling	68477-31-6			1, 4
Distillates, petroleum, heavy arom.	67891-79-6			1, 4
Distillates, petroleum, hydrodesulfurized light catalytic cracked	68333-25-5			1
Distillates, petroleum, hydrodesulfurized middle	64742-80-9			1

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Distillates, petroleum, hydrotreated heavy naphthenic	64742-52-5			1, 2, 3, 4
Distillates, petroleum, hydrotreated heavy paraffinic	64742-54-7			1, 2, 4
Distillates, petroleum, hydrotreated light	64742-47-8			1, 2, 3, 4, 5, 7, 8
Distillates, petroleum, hydrotreated light naphthenic	64742-53-6			1, 2, 8
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8			8
Distillates, petroleum, hydrotreated middle	64742-46-7			1, 2, 3, 4, 8
Distillates, petroleum, light catalytic cracked	64741-59-9			1, 4
Distillates, petroleum, light hydrocracked	64741-77-1			3
Distillates, petroleum, solvent-dewaxed heavy paraffinic	64742-65-0			1
Distillates, petroleum, solvent-refined heavy naphthenic	64741-96-4			1, 4
Distillates, petroleum, steam-cracked	64742-91-2			1, 4
Distillates, petroleum, straight-run middle	64741-44-2			1, 2, 4
Distillates, petroleum, sweetened middle	64741-86-2			1, 4
Ditallow alkyl ethoxylated amines	71011-04-6			3
D-Lactic acid	10326-41-7	X		1, 4
D-Limonene	5989-27-5	X	X	1, 3, 4, 5, 7, 8
Docusate sodium	577-11-7	X		1
Dodecamethylcyclohexasiloxane	540-97-6			8
Dodecane	112-40-3	X		8
Dodecylbenzene	123-01-3	X		3, 4
Dodecylbenzenesulfonic acid	27176-87-0	X	X	2, 3, 4, 8
Dodecylbenzenesulfonic acid, monoethanolamine salt	26836-07-7	X		1, 4
Edifas B	9004-32-4			2, 3, 4
EDTA, copper salt	12276-01-6			1, 5, 6
Endo-1,4-.beta.-mannanase	37288-54-3			3, 8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Epichlorohydrin	106-89-8	X	X	1, 4, 8
Epoxy resin	25085-99-8			1, 4, 8
Erucic amidopropyl dimethyl betaine	149879-98-1			1, 3
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	44992-01-0	X		3
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-,chloride, polymer with 2-propenamide	69418-26-4			1, 3, 4
Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propen-1-yl)oxy]-, chloride (1:1), polymer with 2-propenamide	35429-19-7			8
Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, methyl sulfate, homopolymer	27103-90-8			8
Ethane	74-84-0	X		2, 5
Ethanol	64-17-5	X		1, 2, 3, 4, 5, 6, 8
Ethanol, 2,2',2''-nitrilotris-, tris(dihydrogen phosphate) (ester), sodium salt	68171-29-9	X		4
Ethanol, 2,2'-iminobis-, N-coco alkyl derivs., N-oxides	61791-47-7			1
Ethanol, 2,2'-iminobis-, N-tallow alkyl derivs.	61791-44-4			1
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues	68909-77-3			4, 8
Ethanol, 2,2-oxybis-, reaction products with ammonia, morpholine derivs. residues, acetates (salts)	68877-16-7			4
Ethanol, 2,2-oxybis-, reaction products with ammonia, morpholine derivs. residues, reaction products with sulfur dioxide	102424-23-7			4
Ethanol, 2-[2-[2-(tridecyloxy)ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	25446-78-0	X		1, 4
Ethanol, 2-amino-, polymer with formaldehyde	34411-42-2			4
Ethanol, 2-amino-, reaction products with ammonia, by-products from, phosphonomethylated	68649-44-5			4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Ethanolamine	141-43-5	**X**		1, 2, 3, 4, 6
Ethoxylated dodecyl alcohol	9002-92-0	**X**		4
Ethoxylated hydrogenated tallow alkylamines	61790-82-7			4
Ethoxylated, propoxylated trimethylolpropane	52624-57-4			3
Ethyl acetate	141-78-6	**X**	**X**	1, 4, 7
Ethyl acetoacetate	141-97-9	**X**		1, 4
Ethyl benzoate	93-89-0	**X**		3
Ethyl lactate	97-64-3	**X**		3
Ethyl salicylate	118-61-6	**X**		3
Ethylbenzene	*100-41-4*	**X**	**X**	*1, 2, 3, 4, 7*
Ethylcellulose	9004-57-3			2
Ethylene	74-85-1	**X**		8
Ethylene glycol	*107-21-1*	**X**	**X**	*1, 2, 3, 4, 6, 7, 8*
Ethylene oxide	75-21-8	**X**	**X**	1, 2, 3, 4
Ethylenediamine	107-15-3	**X**	**X**	2, 4
Ethylenediaminetetraacetic acid	60-00-4	**X**		1, 2, 4
Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	**X**		1, 2, 3, 4
Ethylenediaminetetraacetic acid, diammonium copper salt	67989-88-2			4
Ethylenediaminetetraacetic acid, disodium salt	139-33-3	**X**		1, 3, 4, 8
Ethyne	74-86-2	**X**		7
Fats and Glyceridic oils, vegetable, hydrogenated	68334-28-1			8
Fatty acid, tall oil, hexa esters with sorbitol, ethoxylated	61790-90-7			1, 4
Fatty acids, C 8-18 and C18-unsaturated compounds with diethanolamine	68604-35-3			3
Fatty acids, C14-18 and C16-18-unsatd., distn. residues	70321-73-2			2
Fatty acids, C18-unsatd., dimers	61788-89-4	**X**		2

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Fatty acids, C18-unsatd., dimers, compds. with ethoxylated tall-oil fatty acid-polyethylenepolyamine reaction products	68132-59-2			8
Fatty acids, C18-unsatd., dimers, ethoxylated propoxylated	68308-89-4			8
Fatty acids, coco, ethoxylated	61791-29-5			3
Fatty acids, coco, reaction products with diethylenetriamine and soya fatty acids, ethoxylated, chloromethane-quaternized	68604-75-1			8
Fatty acids, coco, reaction products with ethanolamine, ethoxylated	61791-08-0			3
Fatty acids, tall oil, reaction products with acetophenone, formaldehyde and thiourea	68188-40-9			3
Fatty acids, tall-oil	61790-12-3			1, 2, 3, 4
Fatty acids, tall-oil, reaction products with diethylenetriamine	61790-69-0			1, 4
Fatty acids, tall-oil, reaction products with diethylenetriamine, maleic anhydride, tetraethylenepentamine and triethylenetetramine	68990-47-6			8
Fatty acids, tallow, sodium salts	8052-48-0			1, 3
Fatty acids, vegetable-oil, reaction products with diethylenetriamine	68153-72-0			3
Fatty quaternary ammonium chloride	61789-68-2			1, 4
FD&C Blue no. 1	3844-45-9	**X**		1, 4
FD&C Yellow 5	1934-21-0	**X**		8
FD&C Yellow 6	2783-94-0	**X**		8
Ferric chloride	7705-08-0			1, 3, 4
Ferric sulfate	10028-22-5			1, 4
Ferrous sulfate monohydrate	17375-41-6			2
Ferumoxytol	1309-38-2			8
Fiberglass	65997-17-3			2, 3, 4
Formaldehyde	50-00-0	**X**	**X**	1, 2, 3, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Formaldehyde polymer with 4,1,1-(dimethylethyl)phenol and methyloxirane	29316-47-0			3
Formaldehyde polymer with methyl oxirane, 4-nonylphenol and oxirane	63428-92-2			4, 8
Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	30704-64-4			1, 2, 4, 8
Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane, 4-nonylphenol and oxirane	68188-99-8			8
Formaldehyde, polymer with 4-nonylphenol and oxirane	30846-35-6			1, 4
Formaldehyde, polymer with 4-nonylphenol and phenol	40404-63-5			8
Formaldehyde, polymer with ammonia and phenol	35297-54-2			1, 4
Formaldehyde, polymer with bisphenol A	25085-75-0			4
Formaldehyde, polymer with N1-(2-aminoethyl)-1,2-ethanediamine, benzylated	70750-07-1			8
Formaldehyde, polymer with nonylphenol and oxirane	55845-06-2			4
Formaldehyde, polymers with branched 4-nonylphenol, oxirane and 2-methyloxirane	153795-76-7			1 3
Formaldehyde/ amine	50-00-0_3			1, 2, 3, 4
Formamide	75-12-7	**X**		1, 2, 3, 4
Formic acid	*64-18-6*	**X**	**X**	*1, 2, 3, 4, 6, 7*
Formic acid, potassium salt	590-29-4	**X**		1, 3, 4
Frits, chemicals	65997-18-4			8
Fuel oil, no. 2	68476-30-2			1, 2
Fuels, diesel	68334-30-5			2
Fuels, diesel, no. 2	68476-34-6			2, 4, 8
Fuller's earth	8031-18-3			2
Fumaric acid	110-17-8	**X**		1, 2, 3, 4, 6
Fumes, silica	69012-64-2			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Furfural	98-01-1	X	X	1, 4
Furfuryl alcohol	98-00-0	X		1, 4
Galantamine hydrobromide	69353-21-5	X		8
Gas oils, petroleum, straight-run	64741-43-1			1, 4
Gelatin	9000-70-8			1, 4
Gilsonite	12002-43-6			1, 2, 4
Gluconic acid	133-42-6	X		7
Glutaraldehyde	111-30-8	X		1, 2, 3, 4, 7
Glycerides, C14-18 and C16-18-unsatd. mono- and di-	67701-32-0			8
Glycerol	56-81-5	X		1, 2, 3, 4, 5
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	135-37-5	X		1
Glycine, N-(hydroxymethyl)-, monosodium salt	70161-44-3	X		8
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	5064-31-3	X		1, 2, 3, 4
Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)-, trisodium salt	139-89-9	X		1
Glycolic acid	79-14-1	X		1, 3, 4
Glycolic acid sodium salt	2836-32-0	X		1, 3, 4
Glyoxal	107-22-2	X	X	1, 2, 4
Glyoxylic acid	298-12-4	X		1
Goethite (Fe(OH)O)	1310-14-1			8
Guar gum	9000-30-0			1, 2, 3, 4, 7, 8
Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt	68130-15-4			1, 2, 3, 4, 7
Gypsum ($Ca(SO_4).2H_2O$)	13397-24-5			2, 4
Hematite	1317-60-8			1, 2, 4
Hemicellulase	9012-54-8			1, 2, 3, 4, 5
Hemicellulase enzyme concentrate	9025-56-3			3, 4
Heptane	142-82-5	X		1, 2
Heptene, hydroformylation products, high-boiling	68526-88-5			1, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Hexadecyltrimethylammonium bromide	57-09-0	**X**		1
Hexane	110-54-3	**X**	**X**	5
Hexanedioic acid	124-04-9	**X**	**X**	1, 2, 4, 6
Humic acids, commercial grade	1415-93-6			2
Hydrazine	302-01-2		**X**	8
Hydrocarbons, terpene processing by-products	68956-56-9			1, 3, 4
Hydrochloric acid	7647-01-0			1, 2, 3, 4, 5, 6, 7, 8
Hydrogen fluoride	7664-39-3			1, 2, 4
Hydrogen peroxide	7722-84-1			1, 3, 4
Hydrogen sulfide	7783-06-4			1, 2
Hydroxyethylcellulose	9004-62-0			1, 2, 3, 4
Hydroxylamine hydrochloride	5470-11-1			1, 3, 4
Hydroxylamine sulfate (2:1)	10039-54-0			4
Hydroxypropyl cellulose	9004-64-2			2, 4
Hydroxypropyl guar gum	39421-75-5			1, 3, 4, 5, 6, 8
Hydroxyvalerenic acid	1619-16-5	**X**		8
Hypochlorous acid	7790-92-3			8
Illite	12173-60-3			8
Ilmenite ($FeTiO_3$), conc.	98072-94-7			8
Indole	120-72-9	**X**		2
Inulin, carboxymethyl ether, sodium salt	430439-54-6			1, 4
Iridium oxide	12030-49-8			8
Iron	*7439-89-6*		**X**	*2, 4*
Iron oxide	1332-37-2			1, 4
Iron oxide (Fe_3O_4)	1317-61-9			4
Iron(II) sulfate	7720-78-7			2
Iron(II) sulfate heptahydrate	7782-63-0			1, 2, 3, 4
Iron(III) oxide	1309-37-1			1, 2, 4
Isoascorbic acid	89-65-6	**X**		1, 3, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Isobutane	75-28-5	X		2
Isobutene	115-11-7	X		8
Isooctanol	26952-21-6	X		1, 4, 5
Isopentyl alcohol	123-51-3	X		1, 4
Isopropanol	*67-63-0*	X		*1, 2, 3, 4, 6, 7*
Isopropanolamine dodecylbenzene	42504-46-1	X		1, 3, 4
Isopropylamine	75-31-0	X		1, 4
Isoquinoline	119-65-3	X		8
Isoquinoline, reaction products with benzyl chloride and quinoline	68909-80-8	X		3
Isoquinolinium, 2-(phenylmethyl)-, chloride	35674-56-7	X		3
Isotridecanol, ethoxylated	9043-30-5			1, 3, 4, 8
Kaolin	1332-58-7			1, 2, 4
Kerosine, petroleum, hydrodesulfurized	64742-81-0			1, 2, 4
Kieselguhr	61790-53-2			1, 2, 4
Kyanite	1302-76-7			1, 2, 4
Lactic acid	50-21-5	X		1, 4, 8
Lactose	63-42-3	X		3
Latex 2000 TM	9003-55-8			2, 4
Lauryl hydroxysultaine	13197-76-7	X		1
Lavandula hybrida abrial herb oil	8022-15-9			3
L-Dilactide	4511-42-6	X		1, 4
Lead	*7439-92-1*		X	*1, 4*
Lecithin	8002-43-5			4
L-Glutamic acid	56-86-0	X		8
Lignite	129521-66-0			2
Lignosulfuric acid	8062-15-5			2
Ligroine	8032-32-4			8
Limestone	1317-65-3			1, 2, 3, 4
Linseed oil	8001-26-1			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
L-Lactic acid	79-33-4	**X**		1, 4, 8
Magnesium carbonate (1:1)	7757-69-9			8
Magnesium carbonate (1:x)	546-93-0			1, 3, 4
Magnesium chloride	7786-30-3			1, 2, 4
Magnesium chloride hexahydrate	7791-18-6			4
Magnesium hydroxide	1309-42-8			1, 4
Magnesium iron silicate	19086-72-7			1, 4
Magnesium nitrate	10377-60-3			1, 2, 4
Magnesium oxide	1309-48-4			1, 2, 3, 4
Magnesium peroxide	14452-57-4			1, 4
Magnesium phosphide	12057-74-8			1
Magnesium silicate	1343-88-0			1, 4
Magnesium sulfate	7487-88-9			8
Maleic acid homopolymer	26099-09-2			8
Methanamine-N-methyl polymer with chloromethyl oxirane	25988-97-0			4
Methane	74-82-8	**X**		2, 5
Methanol	*67-56-1*	**X**	**X**	*1, 2, 3, 4, 5, 6, 7, 8*
Methenamine	100-97-0	**X**		1, 2, 4
Methoxyacetic acid	625-45-6	**X**		8
Methyl cellulose	9004-67-5			8
Methyl salicylate	119-36-8	**X**		1, 2, 3, 4, 7
Methyl vinyl ketone	78-94-4	**X**		1, 4
Methylcyclohexane	108-87-2	**X**		1
Methylene bis(thiocyanate)	6317-18-6	**X**		2
Methylenebis(5-methyloxazolidine)	66204-44-2	**X**		2
Methyloxirane polymer with oxirane, mono (nonylphenol) ether, branched	68891-11-2			3
Mica	12001-26-2			1, 2, 4, 6
Mineral oil - includes paraffin oil	8012-95-1		**X**	4, 8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Mineral spirits	64475-85-0			2
Mono- and di- potassium salts of phosphorous acid	13492-26-7			8
Montmorillonite	1318-93-0			2
Morpholine	110-91-8	**X**		1, 2, 4
Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	78-21-7	**X**		8
MT 6	76-31-3			8
Mullite	1302-93-8			1,2, 4, 8
N-(2-Acryloyloxyethyl)-N-benzyl-N,N-dimethylammonium chloride	46830-22-2	**X**		3
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	**X**		8
N,N,N-Trimethyl-2[1-oxo-2-propenyl]oxy ethanaminimum chloride, homopolymer	54076-97-0			3
N,N,N-Trimethyl-3-((1-oxooctadecyl)amino)-1-propanaminium methyl sulfate	19277-88-4	**X**		1
N,N,N-Trimethyloctadecan-1-aminium chloride	112-03-8	**X**		1, 3, 4
N,N'-Dibutylthiourea	109-46-6	**X**		1, 4
N,N-Dimethyldecylamine oxide	2605-79-0	**X**		1, 3, 4
N,N-Dimethylformamide	68-12-2	**X**	**X**	1, 2, 4, 5, 8
N,N-Dimethylmethanamine hydrochloride	593-81-7	**X**		1, 4, 5, 7
N,N-Dimethyl-methanamine-N-oxide	1184-78-7	**X**		3
N,N-dimethyloctadecylamine hydrochloride	1613-17-8	**X**		1, 4
N,N'-Methylenebisacrylamide	110-26-9	**X**		1, 4
Naphtha, petroleum, heavy catalytic reformed	64741-68-0			1, 2, 3, 4
Naphtha, petroleum, hydrotreated heavy	64742-48-9			1, 2, 3, 4, 8
Naphthalene	*91-20-3*	**X**	**X**	*1, 2, 3, 4, 5, 7*
Naphthalenesulfonic acid, bis(1-methylethyl)-	28757-00-8	**X**		1, 3, 4
Naphthalenesulfonic acid, polymer with formaldehyde, sodium salt	9084-06-4			2
Naphthalenesulphonic acid, bis (1-methylethyl)-methyl derivatives	99811-86-6	**X**		1

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Naphthenic acid ethoxylate	68410-62-8	X		4
Navy fuels JP-5	8008-20-6_2			1, 2, 3, 4, 8
Nickel sulfate	7786-81-4			2
Nickel(II) sulfate hexahydrate	10101-97-0			1, 4
Nitriles, tallow, hydrogenated	61790-29-2			4
Nitrilotriacetamide	4862-18-4	X		1, 4, 7
Nitrilotriacetic acid	139-13-9	X	X	1, 4
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	X	X	1, 4
Nitrogen	7727-37-9			1, 2, 3, 4, 6
N-Methyl-2-pyrrolidone	872-50-4	X	X	1, 4
N-Methyldiethanolamine	105-59-9	X		2, 4, 8
N-Methylethanolamine	109-83-1	X		4
N-Methyl-N-hydroxyethyl-N-hydroxyethoxyethylamine	68213-98-9	X		4
N-Oleyl diethanolamide	13127-82-7	X		1, 4
Nonyl nonoxynol-10	9014-93-1			4
Nonylphenol (mixed)	25154-52-3			1, 4
Octamethylcyclotetrasiloxane	556-67-2			8
Octoxynol-9	9036-19-5			1, 2, 3, 4, 8
Oil of eucalyptus	8000-48-4			3
Oil of lemongrass	8007-02-1			3
Oil of rosemary	8000-25-7			3
Oleic acid	112-80-1	X		2, 4
Olivine-group minerals	1317-71-1			4
Orange terpenes	8028-48-6			4
Oxirane, 2-methyl-, polymer with oxirane, ether with (chloromethyl) oxirane polymer with 4,4`-(1-methylidene) bis[phenol]	68036-95-3			8
Oxirane, 2-methyl-, polymer with oxirane, mono(2-ethylhexyl) ether	64366-70-7			8
Oxirane, 2-methyl-, polymer with oxirane, monodecyl ether	37251-67-5			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Oxirane, methyl-, polymer with oxirane, mono-C10-16-alkyl ethers, phosphates	68649-29-6			1, 4
Oxygen	7782-44-7			4
Ozone	10028-15-6			8
Paraffin waxes and Hydrocarbon waxes	8002-74-2			1
Paraformaldehyde	30525-89-4			2
PEG-10 Hydrogenated tallow amine	61791-26-2			1, 3
Pentaethylenehexamine	4067-16-7	**X**		4
Pentane	109-66-0	**X**		2, 5
Pentyl acetate	628-63-7	**X**		3
Pentyl butyrate	540-18-1	**X**		3
Peracetic acid	79-21-0	**X**		8
Perboric acid, sodium salt, monohydrate	10332-33-9			1, 8
Perlite	93763-70-3			4
Petrolatum, petroleum, oxidized	64743-01-7			3
Petroleum	8002-05-9			1, 2
Petroleum distillate hydrotreated light	6742-47-8			8
Phenanthrene	*85-01-8*	**X**		*6*
Phenol	*108-95-2*	**X**	**X**	*1, 2, 4*
Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	68123-18-2			8
Phenol-formaldehyde resin	9003-35-4			1, 2, 4, 7
Phosphine	7803-51-2		**X**	1, 4
Phosphonic acid	13598-36-2			1, 4
Phosphonic acid (dimethylamino(methylene))	29712-30-9	**X**		1
Phosphonic acid, (((2-[(2-hydroxyethyl)(phosphonomethyl)amino)ethyl)imino]bis(methylene))bis-, compd. with 2-aminoethanol	129828-36-0	**X**		1
Phosphonic acid, (1-hydroxyethylidene)bis-, potassium salt	67953-76-8	**X**		4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Phosphonic acid, (1-hydroxyethylidene)bis-, tetrasodium salt	3794-83-0	X		1, 4
Phosphonic acid, [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakis-	15827-60-8	X		1, 2, 4
Phosphonic acid, [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakis-, ammonium salt (1:x)	70714-66-8	X		3
Phosphonic acid, [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakis-, sodium salt	22042-96-2	X		3
Phosphonic acid, [[(phosphonomethyl)imino]bis[6,1-hexanediylnitrilobis(methylene)]]tetrakis-	34690-00-1	X		1, 4, 8
Phosphoric acid	7664-38-2		X	1, 2, 4
Phosphoric acid, aluminium sodium salt	7785-88-8		X	1, 2
Phosphoric acid, ammonium salt (1:3)	10361-65-6			8
Phosphoric acid, diammonium salt	7783-28-0		X	2
Phosphoric acid, mixed decyl and Et and octyl esters	68412-60-2			1
Phosphorous acid	10294-56-1			1
Phthalic anhydride	85-44-9	X	X	1, 4
Pine oils	8002-09-3			1, 2, 4
Pluronic F-127	9003-11-6			1, 3, 4, 8
Policapram (Nylon 6)	25038-54-4			1, 4
Poly (acrylamide-co-acrylic acid), partial sodium salt	62649-23-4			3, 4
Poly(acrylamide-co-acrylic acid)	9003-06-9			4, 8
Poly(lactide)	26680-10-4			1
Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, phosphate	51811-79-1			1, 4
Poly(oxy-1,2-ethanediyl), .alpha.-(octylphenyl)-.omega.-hydroxy-, branched	68987-90-6	X		1, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8			1, 4
Poly(oxy-1,2-ethanediyl), .alpha.-[(9Z)-1-oxo-9-octadecenyl]-.omega.-hydroxy-	9004-96-0			8
Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy-, mono-C10-14-alkyl ethers, phosphates	68585-36-4			8
Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy-, mono-C8-10-alkyl ethers, phosphates	68130-47-2			8
Poly(oxy-1,2-ethanediyl), .alpha.-isodecyl-.omega.-hydroxy-	61827-42-7			8
Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C10-16-alkyl ethers, sodium salts	68585-34-2			8
Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C12-14-alkyl ethers, sodium salts	68891-38-3			1, 4
Poly(oxy-1,2-ethanediyl), alpha-(2,3,4,5-tetramethylnonyl)-omega-hydroxy	68015-67-8			1
Poly(oxy-1,2-ethanediyl), alpha-(nonylphenyl)-omega-hydroxy-,branched, phosphates	68412-53-3			1
Poly(oxy-1,2-ethanediyl), alpha-hexyl-omega-hydroxy	31726-34-8			3, 8
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, (9Z)-9-octadecenoate	56449-46-8			3
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, ether with alpha-fluoro-omega-(2-hydroxyethyl)poly(difluoromethylene) (1:1)	65545-80-4			1
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, ether with D-glucitol (2:1), tetra-(9Z)-9-octadecenoate	61723-83-9			8
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(decyloxy)-, ammonium salt (1:1)	52286-19-8			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(hexyloxy)-, ammonium salt (1:1)	63428-86-4			1, 3, 4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(hexyloxy)-, C6-10-alkyl ethers, ammonium salts	68037-05-8			3, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega--(nonylphenoxy)-	9081-17-8			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(octyloxy)-, ammonium salt (1:1)	52286-18-7			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-hydroxy-, C10-12-alkyl ethers, ammonium salts	68890-88-0			8
Poly(oxy-1,2-ethanediyl), alpha-tridecyl-omega-hydroxy-	24938-91-8			1, 3, 4
Poly(oxy-1,2-ethanediyl), alpha-undecyl-omega-hydroxy-, branched and linear	127036-24-2			1
Poly-(oxy-1,2-ethanediyl)-alpha-undecyl-omega-hydroxy	34398-01-1			1, 3, 4, 8
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy branched	127087-87-0			1, 2, 3, 4
Poly(sodium-p-styrenesulfonate)	25704-18-1			1,4
Poly(tetrafluoroethylene)	9002-84-0			8
Poly[imino(1,6-dioxo-1,6-hexanediyl)imino-1,6-hexanediyl]	32131-17-2			2
Polyacrylamide	9003-05-8			1, 2, 4, 6
Polyacrylate/ polyacrylamide blend	NOCAS_51256			2
Polyacrylic acid, sodium bisulfite terminated	66019-18-9			3
Polyethylene glycol	25322-68-3			1, 2, 3, 4, 7, 8
Polyethylene glycol (9Z)-9-octadecenyl ether	9004-98-2			8
Polyethylene glycol ester with tall oil fatty acid	68187-85-9			1
Polyethylene glycol monobutyl ether	9004-77-7			1, 4
Polyethylene glycol mono-C8-10-alkyl ether sulfate ammonium	68891-29-2			1, 3, 4
Polyethylene glycol nonylphenyl ether	9016-45-9			1, 2, 3, 4, 8
Polyethylene glycol tridecyl ether phosphate	9046-01-9			1, 3, 4
Polyethyleneimine	9002-98-6			4
Polyglycerol	25618-55-7			2
Poly-L-aspartic acid sodium salt	34345-47-6			8
Polyoxyethylene sorbitan trioleate	9005-70-3			3

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Polyoxyethylene(10)nonylphenyl ether	26027-38-3			1, 2, 3, 4, 8
Polyoxyl 15 hydroxystearate	70142-34-6			8
Polyoxypropylenediamine	9046-10-0			1
Polyphosphoric acids, esters with triethanolamine, sodium salts	68131-72-6			1
Polyphosphoric acids, sodium salts	68915-31-1		**X**	1, 4
Polypropylene glycol	25322-69-4			1, 2, 4
Polypropylene glycol glycerol triether, epichlorohydrin, bisphenol A polymer	68683-13-6			1
Polyquaternium 5	26006-22-4			1, 4
Polysorbate 20	9005-64-5			8
Polysorbate 60	9005-67-8			3, 4
Polysorbate 80	9005-65-6			3, 4
Polyvinyl acetate copolymer	9003-20-7			2
Polyvinyl acetate, partially hydrolyzed	304443-60-5			8
Polyvinyl alcohol	9002-89-5			1, 2, 4
Polyvinyl alcohol/polyvinyl acetate copolymer	NOCAS_50147			2
Polyvinylidene chloride	9002-85-1			8
Polyvinylpyrrolidone	9003-39-8			8
Portland cement	65997-15-1			2, 4
Potassium acetate	127-08-2	**X**		1, 3, 4
Potassium aluminum silicate	1327-44-2			5
Potassium antimonate	29638-69-5			1, 4
Potassium bisulfate	7646-93-7			8
Potassium borate	12712-38-8			3
Potassium borate (1:x)	20786-60-1			1, 3
Potassium carbonate sesquihydrate	6381-79-9			5
Potassium chloride	7447-40-7			1, 2, 3, 4, 5, 6, 7
Potassium dichromate	7778-50-9			4
Potassium hydroxide	1310-58-3			1, 2, 3, 4, 6

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Potassium iodide	7681-11-0		X	1, 4
Potassium metaborate	13709-94-9			1, 2, 3, 4, 8
Potassium oleate	143-18-0	X		4
Potassium oxide	12136-45-7			1, 4
Potassium persulfate	7727-21-1			1, 2, 4
Potassium phosphate, tribasic	7778-53-2		X	8
Potassium sulfate	7778-80-5			2
Propane	74-98-6	X		2, 5
Propanol, 1(or 2)-(2-methoxymethylethoxy)-	34590-94-8	X		1, 2, 3, 4
Propargyl alcohol	107-19-7	X	X	1, 2, 3, 4, 5, 6, 7, 8
Propylene carbonate	108-32-7	X		1, 4
Propylene pentamer	15220-87-8	X		1
p-Xylene	106-42-3	X		1, 4
Pyridine, alkyl derivs.	68391-11-7			1, 4
Pyridinium, 1-(phenylmethyl)-, alkyl derivs., chlorides	100765-57-9			4, 8
Pyridinium, 1-(phenylmethyl)-, C7-8-alkyl derivs., chlorides	70914-44-2			6
Pyrimidine	289-95-2	X		2
Pyrrole	109-97-7	X		2
Quartz-alpha (SiO2)	14808-60-7			1, 2, 3, 4, 5, 6, 8
Quaternary ammonium compounds (2-ethylhexyl) hydrogenated tallow alkyl)dimethyl, methyl sulfates	308074-31-9			8
Quaternary ammonium compounds, (oxydi-2,1-ethanediyl)bis[coco alkyldimethyl, dichlorides	68607-28-3			2, 3, 4, 8
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, bis(hydrogenated tallow alkyl)dimethylammonium salt with bentonite	71011-25-1			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with bentonite	68153-30-0			2, 5, 6
Quaternary ammonium compounds, benzyl-C10-16-alkyldimethyl, chlorides	68989-00-4			1, 4
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1		**X**	1, 2, 4, 8
Quaternary ammonium compounds, benzyl-C12-18-alkyldimethyl, chlorides	68391-01-5			8
Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite	68953-58-2			2, 3, 4, 8
Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with hectorite	71011-27-3			2
Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides	68424-95-3	**X**		2
Quaternary ammonium compounds, dicoco alkyldimethyl, chlorides	61789-77-3			1
Quaternary ammonium compounds, pentamethyltallow alkyltrimethylenedi-, dichlorides	68607-29-4			4
Quaternary ammonium compounds, trimethyltallow alkyl, chlorides	8030-78-2			1, 4
Quinaldine	91-63-4	**X**		8
Quinoline	91-22-5	**X**	**X**	2, 4
Raffinates (petroleum)	68514-29-4			5
Raffinates, petroleum, sorption process	64741-85-1			1, 2, 4, 8
Residual oils, petroleum, solvent-refined	64742-01-4			5
Residues, petroleum, catalytic reformer fractionator	64741-67-9			1, 4, 8
Rhodamine B	81-88-9	**X**		4
Rosin	8050-09-7			1, 4
Rutile titanium dioxide	1317-80-2			8
Sand	308075-07-2			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Scandium oxide	12060-08-1			8
Sepiolite	63800-37-3			2
Silane, dichlorodimethyl-, reaction products with silica	68611-44-9			2, 4
Silica	*7631-86-9*			*1, 2, 3, 4, 8*
silica gel, cryst. -free	112926-00-8			3, 4
Silica, amorphous, fumed, cryst.-free	112945-52-5			1, 3, 4
Silica, vitreous	60676-86-0			1, 4, 8
Silicic acid, aluminum potassium sodium salt	12736-96-8			4
Siloxanes (Polysiloxane)	9011-19-2			4
Siloxanes and Silicones, di-Me, 3-hydroxypropyl Me, ethoxylated propoxylated	68937-55-3			8
Siloxanes and Silicones, di-Me, Me hydrogen	68037-59-2			8
Siloxanes and silicones, di-Me, polymers with Me silsesquioxanes	68037-74-1			4
Siloxanes and Silicones, di-Me, reaction products with silica	67762-90-7			4
Siloxanes and silicones, dimethyl,	63148-52-7			4
Silwet L77	27306-78-1			1
Sodium 1-octanesulfonate	5324-84-5	**X**		3
Sodium 2-mercaptobenzothiolate	2492-26-4	**X**		2
Sodium acetate	127-09-3	**X**		1, 3, 4
Sodium aluminate	1302-42-7			2, 4
Sodium benzoate	532-32-1	**X**		3
Sodium bicarbonate	144-55-8	**X**		1, 2, 3, 4, 7
Sodium bis(tridecyl) sulfobutanedioate	2673-22-5	**X**		4
Sodium bisulfite	7631-90-5			1, 3, 4
Sodium borate	1333-73-9			1, 4, 6, 7
Sodium bromate	7789-38-0			1, 2, 4
Sodium bromide	7647-15-6			1, 2, 3, 4, 7
Sodium bromosulfamate	1004542-84-0			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Sodium C14-16 alpha-olefin sulfonate	68439-57-6	X		1, 3, 4
Sodium caprylamphopropionate	68610-44-6	X		4
Sodium carbonate	497-19-8	X		1, 2, 3, 4, 8
Sodium chlorate	7775-09-9		X	1, 4
Sodium chloride	7647-14-5			1, 2, 3, 4, 5, 8
Sodium chlorite	7758-19-2		X	1, 2, 3, 4, 5, 8
Sodium chloroacetate	3926-62-3	X		3
Sodium cocaminopropionate	68608-68-4			1
Sodium decyl sulfate	142-87-0	X		1
Sodium D-gluconate	527-07-1	X		4
Sodium diacetate	126-96-5	X		1, 4
Sodium dichloroisocyanurate	2893-78-9	X		2
Sodium dl-lactate	72-17-3	X		8
Sodium dodecyl sulfate	151-21-3	X		8
Sodium erythorbate (1:1)	6381-77-7	X		1, 3, 4, 8
Sodium ethasulfate	126-92-1	X		1
Sodium formate	141-53-7	X		2, 8
Sodium hydrogen sulfate	7681-38-1			4
Sodium hydroxide	1310-73-2			1, 2, 3, 4, 7, 8
Sodium hydroxymethanesulfonate	870-72-4	X		8
Sodium hypochlorite	7681-52-9			1, 2, 3, 4, 8
Sodium iodide	7681-82-5		X	4
Sodium ligninsulfonate	8061-51-6			2
Sodium l-lactate	867-56-1	X		8
Sodium maleate (1:x)	18016-19-8	X		8
Sodium metabisulfite	7681-57-4			1
Sodium metaborate	7775-19-1			3, 4
Sodium metaborate dihydrate	16800-11-6			1, 4
Sodium metaborate tetrahydrate	10555-76-7			1, 4, 8
Sodium metasilicate	6834-92-0			1, 2, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Sodium molybdate(VI)	7631-95-0			8
Sodium nitrate	7631-99-4			2
Sodium nitrite	7632-00-0			1, 2, 4
Sodium N-methyl-N-oleoyltaurate	137-20-2	X		4
Sodium octyl sulfate	142-31-4	X		1
Sodium oxide	1313-59-3			1
Sodium perborate	11138-47-9			4
Sodium perborate tetrahydrate	10486-00-7			1, 4, 5, 8
Sodium peroxoborate	7632-04-4			1
Sodium persulfate	7775-27-1			1, 2, 3, 4, 7, 8
Sodium phosphate	7632-05-5			1, 4
Sodium polyacrylate	9003-04-7			1, 2, 3, 4
Sodium pyrophosphate	7758-16-9		X	1, 2, 4
Sodium salicylate	54-21-7	X		1, 4
Sodium sesquicarbonate	533-96-0	X		1, 2
Sodium silicate	1344-09-8			1, 2, 4
Sodium starch glycolate	9063-38-1			2
Sodium sulfate	7757-82-6			1, 2, 3, 4
Sodium sulfite	7757-83-7			2, 4, 8
Sodium thiocyanate	540-72-7	X		1, 4
Sodium thiosulfate	7772-98-7			1, 2, 3, 4
Sodium thiosulfate, pentahydrate	10102-17-7			1, 4
Sodium trichloroacetate	650-51-1	X		1, 4
Sodium trimetaphosphate	7785-84-4		X	8
Sodium xylenesulfonate	1300-72-7	X		1, 3, 4
Sodium zirconium lactate	15529-67-6			8
Sodium zirconium lactic acid (4:4:1)	10377-98-7			1, 4
Solvent naphtha, petroleum, heavy aliph.	64742-96-7			2, 4, 8
Solvent naphtha, petroleum, heavy arom.	64742-94-5			1, 2, 4, 5, 8
Solvent naphtha, petroleum, light aliph.	64742-89-8			8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Solvent naphtha, petroleum, light arom.	64742-95-6			1, 2, 4
Sorbic acid	110-44-1	**X**		8
Sorbitan sesquioleate	8007-43-0	**X**		4
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	**X**		1, 2, 3, 4
Sorbitan, monooctadecanoate	1338-41-6	**X**		8
Sorbitan, tri-(9Z)-9-octadecenoate	26266-58-0	**X**		8
Spirit of ammonia, aromatic	8013-59-0			8
Stannous chloride dihydrate	10025-69-1			1, 4
Starch	9005-25-8			1, 2, 4
Steam cracked distillate, cyclodiene dimer, dicyclopentadiene polymer	68131-87-3			1
Stoddard solvent	8052-41-3			1, 3, 4
Stoddard solvent IIC	64742-88-7			1, 2, 4
Strontium chloride	10476-85-4		**X**	4
Styrene	100-42-5	**X**	**X**	2
Subtilisin	9014-01-1			8
Sucrose	57-50-1	**X**		1, 2, 3, 4
Sulfamic acid	5329-14-6			1, 4
Sulfan blue	129-17-9	**X**		8
Sulfate	*14808-79-8*			*1, 4*
Sulfo NHS Biotin	119616-38-5			8
Sulfomethylated quebracho	68201-64-9			2
Sulfonic acids, C10-16-alkane, sodium salts	68608-21-9			6
Sulfonic acids, petroleum	61789-85-3			1
Sulfonic acids, petroleum, sodium salts	68608-26-4			3
Sulfur dioxide	7446-09-5			2, 4, 8
Sulfuric acid	7664-93-9			1, 2, 4, 7
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	68955-19-1	**X**		4
Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	68187-17-7	**X**		1, 4, 8

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Symclosene	87-90-1	X		2
Talc	14807-96-6			1, 3, 4, 6, 7
Tall oil	8002-26-4			4, 8
Tall oil imidazoline	61791-36-4			4
Tall oil, compound with diethanolamine	68092-28-4			1
Tall oil, ethoxylated	65071-95-6			4, 8
Tall-oil pitch	8016-81-7			4
Tallow alkyl amines acetate	61790-60-1			8
Tar bases, quinoline derivatives, benzyl chloride-quaternized	72480-70-7			1, 3, 4
Tegin M	8043-29-6			8
Terpenes and Terpenoids, sweet orange-oil	68647-72-3			1, 3, 4, 8
Terpineol	8000-41-7			1, 3
tert-Butyl hydroperoxide	75-91-2	X		1, 4
tert-Butyl perbenzoate	614-45-9	X		1
Tetra-calcium-alumino-ferrite	12068-35-8			1, 2, 4
Tetradecane	629-59-4	X		8
Tetradecyldimethylbenzylammonium chloride	139-08-2	X		1, 4, 8
Tetraethylene glycol	112-60-7	X		1, 4
Tetraethylenepentamine	112-57-2	X		1, 4
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	X		1, 2, 3, 4, 7
Tetramethyl orthosilicate	681-84-5			1
Tetramethylammonium chloride	75-57-0	X		1, 2, 3, 4, 7, 8
Tetrasodium pyrophosphate	7722-88-5		X	8
Thiamine hydrochloride	67-03-8	X		8
Thiocyanic acid, ammonium salt	1762-95-4	X		2, 3, 4
Thioglycolic acid	68-11-1	X		1, 2, 3, 4
Thiourea	62-56-6	X	X	1, 2, 3, 4, 6
Thiourea, polymer with formaldehyde and 1-phenylethanone	68527-49-1			1, 4, 8
Thuja plicata donn ex. D. don leaf oil	68917-35-1			3

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Tin(II) chloride	7772-99-8			1
Titanium dioxide	13463-67-7			1, 2, 4
Titanium(4+) 2-[bis(2-hydroxyethyl)amino]ethanolate propan-2-olate (1:2:2)	36673-16-2			1
Titanium, isopropoxy (triethanolaminate)	74665-17-1			1, 4
Toluene	*108-88-3*	**X**	**X**	*1, 3, 4*
Tributyl phosphate	126-73-8	**X**	**X**	1, 2, 4
Tributyltetradecylphosphonium chloride	81741-28-8	**X**		1, 3, 4
Tricalcium phosphate	7758-87-4		**X**	1, 4
Tricalcium silicate	12168-85-3			1, 2, 4
Tridecane	629-50-5	**X**		8
Triethanolamine	102-71-6	**X**		1, 2, 4
Triethanolamine hydrochloride	637-39-8	**X**		8
Triethanolamine hydroxyacetate	68299-02-5	**X**		3
Triethanolamine polyphosphate ester	68131-71-5			1, 4, 8
Triethyl citrate	77-93-0	**X**		1, 4
Triethyl phosphate	78-40-0	**X**		1, 4
Triethylene glycol	112-27-6	**X**		1, 2, 3
Triethylenetetramine	112-24-3	**X**		4
Triisopropanolamine	122-20-3	**X**		1, 4
Trimethanolamine	14002-32-5	**X**		3
Trimethyl borate	121-43-7			8
Trimethylamine	75-50-3	**X**		8
Trimethylamine quaternized polyepichlorohydrin	51838-31-4			1, 2, 3, 4, 5, 8
Trimethylbenzene	25551-13-7			1, 2, 4
Triphosphoric acid, pentasodium salt	7758-29-4		**X**	1, 4
Tripoli	1317-95-9			4
Tripotassium citrate monohydrate	6100-05-6	**X**		4
Tripropylene glycol monomethyl ether	25498-49-1	**X**		2

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Trisodium citrate	68-04-2	**X**		3
Trisodium citrate dihydrate	6132-04-3	**X**		1, 4
Trisodium ethylenediaminetetraacetate	150-38-9	**X**		1, 3
Trisodium ethylenediaminetriacetate	19019-43-3	**X**		1, 4, 8
Trisodium phosphate	7601-54-9		**X**	1, 2, 4
Trisodium phosphate dodecahydrate	10101-89-0			1
Tritan R (X-100)	92046-34-9			8
Triton X-100	9002-93-1			1, 3, 4
Tromethamine	77-86-1	**X**		3, 4
Tryptone	73049-73-7			8
Ulexite	1319-33-1			1, 2, 3, 8
Undecane	1120-21-4	**X**		3, 8
Undecanol, branched and linear	128973-77-3			8
Urea	57-13-6	**X**		1, 2, 4, 8
Vermiculite	1318-00-9			2
Vinyl acetate ethylene copolymer	24937-78-8			1, 4
Vinylidene chloride/methylacrylate copolymer	25038-72-6			4
Water	7732-18-5			2, 4, 8
White mineral oil, petroleum	8042-47-5			1, 2, 4
Xylenes	*1330-20-7*	**X**	**X**	*1, 2, 4*
Yeast extract	8013-01-2			8
Zeolites	1318-02-1			8
Zinc	*7440-66-6*		**X**	*2*
Zinc carbonate	3486-35-9			2
Zinc chloride	7646-85-7			1, 2
Zinc oxide	1314-13-2			1, 4
Zinc sulfate monohydrate	7446-19-7			8
Zirconium nitrate	13746-89-9			2, 6
Zirconium oxide sulfate	62010-10-0			1, 4
Zirconium oxychloride	7699-43-6			1, 2, 4

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Zirconium(IV) chloride tetrahydrofuran complex	21959-01-3			5
Zirconium(IV) sulfate	14644-61-2			2, 6
Zirconium, 1,1'-((2-((2-hydroxyethyl)(2-hydroxypropyl)amino)ethyl)imino)bis(2-propanol) complexes	197980-53-3			4
Zirconium, acetate lactate oxo ammonium complexes	68909-34-2			4, 8
Zirconium, chloro hydroxy lactate oxo sodium complexes	174206-15-6			4
Zirconium, hydroxylactate sodium complexes	113184-20-6			1, 4
Zirconium,tetrakis[2-[bis(2-hydroxyethyl)amino-kN]ethanolato-kO]-	101033-44-7			1, 2, 4, 5

Table A-3. List of generic names of chemicals reportedly used in hydraulic fracturing fluids.

In some cases, the generic chemical name masks a specific chemical name and CASRN provided to the EPA and claimed as CBI by one or more of the nine hydraulic fracturing service companies.

Generic chemical name	Reference
2-Substituted aromatic amine salt	1, 4
Acetylenic alcohol	1
Acrylamide acrylate copolymer	4
Acrylamide copolymer	1, 4
Acrylamide modified polymer	4
Acrylamide-sodium acrylate copolymer	4
Acrylate copolymer	1
Acrylic copolymer	1
Acrylic polymer	1, 4
Acrylic resin	4
Acyclic hydrocarbon blend	1, 4
Acylbenzylpyridinium choride	8
Alcohol alkoxylate	1, 4
Alcohol and fatty acid blend	2

Generic chemical name	Reference
Alcohol ethoxylates	4
Alcohols	1, 4
Alcohols, C9-C22	1, 4
Aldehydes	1, 4, 5
Alfa-alumina	1, 4
Aliphatic acids	1, 2, 3, 4
Aliphatic alcohol	2
Aliphatic alcohol glycol ether	3, 4
Aliphatic alcohols, ethoxylated	2
Aliphatic amine derivative	1
Aliphatic carboxylic acid	4
Alkaline bromide salts	1, 4
Alkaline metal oxide	4
Alkanes/alkenes	4
Alkanolamine derivative	2
Alkanolamine/aldehyde condensate	1, 2, 4
Alkenes	1, 4
Alklaryl sulfonic acid	1, 4
Alkoxylated alcohols	1
Alkoxylated amines	1, 4
Alkyaryl sulfonate	1, 2, 3, 4
Alkyl alkoxylate	1, 4
Alkyl amide	4
Alkyl amine	1, 4
Alkyl amine blend in a metal salt solution	1, 4
Alkyl aryl amine sulfonate	4
Alkyl aryl polyethoxy ethanol	3, 4
Alkyl dimethyl benzyl ammonium chloride	4
Alkyl esters	1, 4
Alkyl ether phosphate	4
Alkyl hexanol	1, 4
Alkyl ortho phosphate ester	1, 4

Generic chemical name	Reference
Alkyl phosphate ester	1, 4
Alkyl phosphonate	4
Alkyl pyridines	2
Alkyl quaternary ammonium chlorides	1, 4
Alkyl quaternary ammonium salt	4
Alkylamine alkylaryl sulfonate	4
Alkylamine salts	2
Alkylaryl sulfonate	1, 4
Alkylated quaternary chloride	1, 2, 4
Alkylated sodium naphthalenesulphonate	2
Alkylbenzenesulfonate	2
Alkylbenzenesulfonic acid	1, 4, 5
Alkylethoammonium sulfates	1
Alkylphenol ethoxylates	1, 4
Alkylpyridinium quaternary	4
Alphatic alcohol polyglycol ether	2
Aluminum oxide	1, 4
Amide	4
Amidoamine	1, 4
Amine	1, 4
Amine compound	4
Amine oxides	1, 4
Amine phosphonate	1, 4
Amine salt	1
Amino compounds	1, 4
Amino methylene phosphonic acid salt	1, 4
Ammonium alcohol ether sulfate	1, 4
Ammonium salt	1, 4
Ammonium salt of ethoxylated alcohol sulfate	1, 4
Amorphous silica	4
Amphoteric surfactant	2
Anionic acrylic polymer	2

Generic chemical name	Reference
Anionic copolymer	1, 4
Anionic polyacrylamide	1, 2, 4
Anionic polyacrylamide copolymer	1, 4, 6
Anionic polymer	1, 3, 4
Anionic surfactants	2, 4, 6
Antifoulant	1, 4
Antimonate salt	1, 4
Aqueous emulsion of diethylpolysiloxane	2
Aromatic alcohol glycol ether	1
Aromatic aldehyde	1, 4
Aromatic hydrocarbons	3, 4
Aromatic ketones	1, 2, 3, 4
Aromatic polyglycol ether	1
Arsenic compounds	4
Ashes, residues	4
Bentone clay	4
Biocide	4
Biocide component	1, 4
Bis-quaternary methacrylamide monomer	4
Blast furnace slag	4
Borate salts	1, 2, 4
Cadmium compounds	4
Carbohydrates	1, 2, 4
Carboxylmethyl hydroxypropyl guar	4
Cationic polyacrylamide	4
Cationic polymer	2, 4
Cedar fiber, processed	2
Cellulase enzyme	1
Cellulose derivative	1, 2, 4
Cellulose ether	2
Cellulosic polymer	2
Ceramic	4

Generic chemical name	Reference
Chlorous ion solution	1
Chromates	1, 4
Chrome-free lignosulfonate compound	2
Citrus rutaceae extract	4
Common white	4
Complex alkylaryl polyo-ester	1
Complex aluminum salt	1, 4
Complex carbohydrate	2
Complex organometallic salt	1
Complex polyamine salt	7
Complex substituted keto-amine	1
Complex substituted keto-amine hydrochloride	1
Copper compounds	6
Coric oxide	4
Cotton dust (raw)	2
Cottonseed hulls	2
Cured acrylic resin	1, 4
Cured resin	1, 4, 5
Cured urethane resin	1, 4
Cyclic alkanes	1, 4
Defoamer	4
Dibasic ester	4
Dicarboxylic acid	1, 4
Diesel	1, 4, 6
Dimethyl silicone	1, 4
Dispersing agent	1
Emulsifier	4
Enzyme	4
Epoxy	4
Epoxy resin	1, 4
Essential oils	1, 4
Ester Salt	2, 4

Generic chemical name	Reference
Esters	2, 4
Ether compound	4
Ether salt	4
Ethoxylated alcohol blend	4
Ethoxylated alcohol/ester mixture	4
Ethoxylated alcohols	1, 2, 4, 5, 7
Ethoxylated alkyl amines	1, 4
Ethoxylated amine blend	4
Ethoxylated amines	1, 4
Ethoxylated fatty acid	4
Ethoxylated fatty acid ester	1, 4
Ethoxylated nonionic surfactant	1, 4
Ethoxylated nonylphenol	1, 2, 4
Ethoxylated sorbitol esters	1, 4
Ethylene oxide-nonylphenol polymer	4
Fatty acid amine salt mixture	4
Fatty acid ester	1, 2, 4
Fatty acid tall oil	1, 4
Fatty acid, ethoxylate	4
Fatty acids	1
Fatty alcohol alkoxylate	1, 4
Fatty alkyl amine salt	1, 4
Fatty amine carboxylates	1, 4
Fatty imidazoline	4
Fluoroaliphatic polymeric esters	1, 4
Formaldehyde polymer	1
Glass fiber	1, 4
Glyceride esters	2
Glycol	4
Glycol blend	2
Glycol ethers	1, 4, 7
Ground cedar	2

Generic chemical name	Reference
Ground paper	2
Guar derivative	1, 4
Guar gum	4
Haloalkyl heteropolycycle salt	1, 4
Hexanes	1
High molecular weight polymer	2
High pH conventional enzymes	2
Hydrocarbons	1
Hydrogen solvent	4
Hydrotreated and hydrocracked base oil	1, 4
Hydrotreated distillate, light C9-16	4
Hydrotreated heavy naphthalene	5
Hydrotreated light distillate	2, 4
Hydrotreated light petroleum distillate	4
Hydroxyalkyl imino carboxylic sodium salt	2
Hydroxycellulose	6
Hydroxyethyl cellulose	1, 2, 4
Imidazolium compound	4
Inner salt of alkyl amines	1, 4
Inorganic borate	1, 4
Inorganic chemical	4
Inorganic particulate	1, 4
Inorganic salt	2, 4
Iso-alkanes/n-alkanes	1, 4
Isomeric aromatic ammonium salt	1, 4
Latex	2, 4
Lead compounds	4
Low toxicity base oils	1, 4
Lubra-Beads course	4
Maghemite	1, 4
Magnetite	1, 4
Metal salt	1

Generic chemical name	Reference
Metal salt solution	1
Mineral	1, 4
Mineral fiber	2
Mineral filler	1
Mineral oil	4
Mixed titanium ortho ester complexes	1, 4
Modified acrylamide copolymer	2, 4
Modified acrylate polymer	4
Modified alkane	1, 4
Modified bentonite	4
Modified cycloaliphatic amine adduct	1, 4
Modified lignosulfonate	2, 4
Naphthalene derivatives	1, 4
Neutralized alkylated napthalene sulfonate	4
Nickel chelate catalyst	4
Nonionic surfactant	1
N-tallowalkyltrimethylenediamines	4
Nuisance particulates	1, 2, 4
Nylon	4
Olefinic sulfonate	1, 4
Olefins	1, 4
Organic acid salt	1, 4
Organic acids	1, 4
Organic alkyl amines	4
Organic chloride	4
Organic modified bentonite clay	4
Organic phosphonate	1, 4
Organic phosphonate salts	1, 4
Organic phosphonic acid salts	1, 4
Organic polymer	4
Organic polyol	4
Organic salt	1, 4

Generic chemical name	Reference
Organic sulfur compound	1, 4
Organic surfactants	1
Organic titanate	1, 4
Organo amino silane	4
Organo phosphonic acid	4
Organo phosphonic acid salt	4
Organometallic ammonium complex	1
Organophilic clay	4
Oxidized tall oil	2
Oxoaliphatic acid	2
Oxyalkylated alcohol	1, 4
Oxyalkylated alkyl alcohol	2, 4
Oxyalkylated alkylphenol	1, 2, 3, 4
Oxyalkylated fatty acid	1, 4
Oxyalkylated fatty alcohol salt	2
Oxyalkylated phenol	1, 4
Oxyalkylated phenolic resin	4
Oxyalkylated polyamine	1
Oxyalkylated tallow diamine	2
Oxyethylated alcohol	2
Oxylated alcohol	1, 4
P/F resin	4
Paraffin inhibitor	4
Paraffinic naphthenic solvent	1
Paraffinic solvent	1, 4
Paraffins	1
Pecan shell	2
Petroleum distallate blend	2, 3, 4
Petroleum gas oils	1
Petroleum hydrocarbons	4
Petroleum solvent	2
Phosphate ester	1, 4

Generic chemical name	Reference
Phosphonate	2
Phosphonic acid	1, 4
Phosphoric acid, mixed polyoxyalkylene aryl and alkyl esters	4
Plasticizer	1, 2
Polyacrylamide copolymer	4
Polyacrylamides	1
Polyacrylate	1, 4
Polyactide resin	4
Polyalkylene esters	4
Polyaminated fatty acid	2
Polyaminated fatty acid surfactants	2
Polyamine	1, 4
Polyamine polymer	4
Polyanionic cellulose	1
Polyaromatic hydrocarbons	6
Polycyclic organic matter	6
Polyelectrolyte	4
Polyether polyol	2
Polyethoxylated alkanol	2, 3, 4
Polyethylene copolymer	4
Polyethylene glycols	4
Polyethylene wax	4
Polyglycerols	2
Polyglycol	2
Polyglycol ether	6
Polylactide resin	4
Polymer	2, 4
Polymeric hydrocarbons	3, 4
Polymerized alcohol	4
Polymethacrylate polymer	4
Polyol phosphate ester	2
Polyoxyalkylene phosphate	2

Generic chemical name	Reference
Polyoxyalkylene sulfate	2
Polyoxyalkylenes	1, 4, 7
Polyphenylene ether	4
Polyphosphate	4
Polypropylene glycols	2
Polyquaternary amine	4
Polysaccaride polymers in suspension	2
Polysaccharide	4
Polysaccharide blend	4
Polyvinylalcohol/polyvinylactetate copolymer	4
Potassium chloride substitute	4
Quarternized heterocyclic amines	4
Quaternary amine	2, 4
Quaternary amine salt	4
Quaternary ammonium chloride	4
Quaternary ammonium compound	1, 2, 4
Quaternary ammonium salts	1, 2, 4
Quaternary compound	1, 4
Quaternary salt	1, 4
Quaternized alkyl nitrogenated compd	4
Red dye	4
Refined mineral oil	2
Resin	4
Salt of amine-carbonyl condensate	3, 4
Salt of fatty acid/polyamine reaction product	3, 4
Salt of phosphate ester	1
Salt of phosphono-methylated diamine	1, 4
Salts	4
Salts of oxyalkylated fatty amines	4
Sand	4
Sand, AZ silica	4
Sand, brown	4

Generic chemical name	Reference
Sand, sacked	4
Sand, white	4
Secondary alcohol	1, 4
Silica sand, 100 mesh, sacked	4
Silicone emulsion	1
Silicone ester	4
Sodium acid pyrophosphate	4
Sodium calcium magnesium polyphosphate	4
Sodium phosphate	4
Sodium salt of aliphatic amine acid	2
Sodium xylene sulfonate	4
Softwood dust	2
Starch blends	6
Substituted alcohol	1, 2, 4
Substituted alkene	1
Substituted alklyamine	1, 4
Substituted alkyne	4
Sulfate	4
Sulfomethylated tannin	2, 5
Sulfonate	4
Sulfonate acids	1
Sulfonate surfactants	1
Sulfonated asphalt	2
Sulfonic acid salts	1, 4
Sulfur compound	1, 4
Sulphonic amphoterics	4
Sulphonic amphoterics blend	4
Surfactant blend	3, 4
Surfactants	1, 2, 4
Synthetic copolymer	2
Synthetic polymer	4
Tallow soap	4

Generic chemical name	Reference
Telomer	4
Terpenes	1, 4
Titanium complex	4
Triethanolamine zirconium chelate	1 4
Triterpanes	4
Vanadium compounds	4
Wall material	1
Walnut hulls	1, 2, 4
Zirconium complex	2, 4
Zirconium salt	4

Table A-4. Chemicals detected in flowback or produced water.

An "X" indicates the availability of physicochemical properties from EPI Suite™ and selected toxicity reference values (see Appendix G). An empty cell indicates no information was available from the sources we consulted. Reference number corresponds to the citations in Table A-1. Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1,2,3-Trichlorobenzene	87-61-6	**X**	**X**	3, 9
1,2,4-Trichlorobenzene	120-82-1	**X**	**X**	9
1,2,4-Trimethylbenzene	*95-63-6*	**X**		*3, 9, 10*
1,2-Propylene glycol	*57-55-6*	**X**	**X**	*3, 9*
1,3,5-Trimethylbenzene	*108-67-8*	**X**		*3, 9, 10*
1,4-Dioxane	*123-91-1*	**X**	**X**	*9, 10*
2,4-Dimethylphenol	105-67-9	**X**	**X**	3, 9, 10
2,6-Dichlorophenol	87-65-0	**X**		3, 9
2-Methylnaphthalene	91-57-6	**X**	**X**	3, 9, 10
2-Methylpropanoic acid	79-31-2	**X**		10
2-Methylpyridine	109-06-8	**X**		3, 9
7,12-Dimethylbenz(a)anthracene	57-97-6	**X**	**X**	3, 9
Acetic acid	*64-19-7*	**X**		*3, 9, 10*

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Acetone	*67-64-1*	**X**	**X**	*3, 9, 10*
Acetophenone	*98-86-2*	**X**	**X**	*3, 9*
Acrolein	*107-02-8*	**X**	**X**	*9*
Acrylonitrile	107-13-1	**X**	**X**	3, 9
Aldrin	309-00-2	**X**	**X**	3, 9
Aluminum	*7429-90-5*		**X**	*3, 9, 10*
Ammonia	*7664-41-7*			*3, 9, 10*
Antimony	7440-36-0		**X**	3, 9, 10
Aroclor 1248	12672-29-6	**X**		3, 9
Arsenic	*7440-38-2*		**X**	*3, 9, 10*
Barium	7440-39-3		**X**	3, 9, 10
Benzene	*71-43-2*	**X**	**X**	*3, 9, 10*
Benzo(a)pyrene	50-32-8	**X**	**X**	3, 9
Benzo(b)fluoranthene	205-99-2	**X**	**X**	3, 9
Benzo(g,h,i)perylene	191-24-2	**X**		3, 9, 10
Benzo(k)fluoranthene	207-08-9	**X**	**X**	3, 9
Benzyl alcohol	100-51-6	**X**	**X**	3, 9, 10
Beryllium	7440-41-7		**X**	3, 9, 10
beta-Hexachlorocyclohexane	319-85-7	**X**	**X**	3, 9
Bis(2-chloroethyl) ether	*111-44-4*	**X**	**X**	*3, 9*
Boron	7440-42-8		**X**	3, 9, 10
Bromide	24959-67-9			3, 9, 10
Bromodichloromethane	75-27-4	**X**	**X**	3
Bromoform	75-25-2	**X**	**X**	3, 9, 10
Butanoic acid	107-92-6	**X**		9, 10
Butylbenzene	104-51-8	**X**	**X**	9, 10
Cadmium	7440-43-9		**X**	3, 9, 10
Caesium-137	10045-97-3			3
Calcium	7440-70-2			3, 9, 10
Carbon dioxide	*124-38-9*	**X**		*3, 9, 10*

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Carbon disulfide	75-15-0	X	X	3, 9
Chloride	*16887-00-6*			*3, 9, 10*
Chlorine	*7782-50-5*		X	*3, 10*
Chlorodibromomethane	124-48-1	X	X	3
Chloroform	67-66-3	X	X	3, 9, 10
Chloromethane	74-87-3	X		3, 10
Chromium	7440-47-3			3, 9, 10
Chromium (III)	*16065-83-1*		X	*3*
Chromium (VI)	*18540-29-9*		X	*3, 10*
Cobalt	7440-48-4		X	3, 9, 10
Copper	*7440-50-8*		X	*3, 9, 10*
Cumene	*98-82-8*	X	X	*3, 9*
Cyanide	57-12-5	X	X	3, 9, 10
delta-Hexachlorocyclohexane	319-86-8	X		9
Di(2-ethylhexyl) phthalate	*117-81-7*	X	X	*3, 9, 10*
Dibenz(a,h)anthracene	53-70-3	X	X	3, 9
Dibutyl phthalate	84-74-2	X	X	3, 9, 10
Dichloromethane	*75-09-2*	X	X	*9, 10*
Dieldrin	60-57-1	X	X	9
Diethyl phthalate	84-66-2	X	X	9
Dioctyl phthalate	117-84-0	X	X	9, 10
Diphenylamine	122-39-4	X	X	3, 9
Endosulfan I	959-98-8	X		3, 9
Endosulfan II	33213-65-9	X		3, 9
Endrin aldehyde	7421-93-4	X		3, 9
Ethylbenzene	*100-41-4*	*X*	*X*	*3, 9, 10*
Ethylene glycol	*107-21-1*	*X*	*X*	*3, 9*
Fluoranthene	206-44-0	X	X	3, 9
Fluorene	86-73-7	X	X	3, 9, 10
Fluoride	16984-48-8			3, 9, 10

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Formic acid	*64-18-6*	***X***	***X***	*10*
Heptachlor	76-44-8	**X**	**X**	3, 9
Heptachlor epoxide	1024-57-3	**X**	**X**	3, 9
Heptanoic acid	111-14-8	**X**		10
Hexanoic acid	142-62-1	**X**		10
Indeno(1,2,3-cd)pyrene	193-39-5	**X**	**X**	3, 9
Iron	*7439-89-6*		***X***	*3, 9, 10*
Isopropanol	*67-63-0*	***X***		*3, 9*
Isovaleric acid	503-74-2	**X**		10
Lead	*7439-92-1*		***X***	*3, 9, 10*
Lindane	58-89-9	**X**	**X**	3, 9
Lithium	7439-93-2		**X**	3, 9, 10
Magnesium	7439-95-4			3, 9, 10
Manganese	7439-96-5		**X**	3, 9, 10
m-Cresol	108-39-4	**X**	**X**	3, 9, 10
Mercury	7439-97-6		**X**	3, 9, 10
Methanol	*67-56-1*	***X***	***X***	*3, 9*
Methyl bromide	74-83-9	**X**	**X**	3, 9
Methyl ethyl ketone	78-93-3	**X**	**X**	3, 9, 10
Molybdenum	7439-98-7		**X**	3, 9, 10
Naphthalene	*91-20-3*	***X***	***X***	*3, 9, 10*
Nickel	7440-02-0			3, 9, 10
Nitrate	14797-55-8		**X**	3, 9, 10
Nitrite	14797-65-0		**X**	3, 9, 10
N-Nitrosodiphenylamine	86-30-6	**X**	**X**	3, 9
o-Cresol	95-48-7	**X**	**X**	3, 9, 10
p,p'-DDE	72-55-9	**X**	**X**	3, 9
p-Cresol	106-44-5	**X**	**X**	3, 9, 10
p-Cymene	99-87-6	**X**		9, 10
Pentanoic acid	109-52-4	**X**		10

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Phenanthrene	*85-01-8*	***X***		*3, 9, 10*
Phenol	*108-95-2*	***X***	***X***	*3, 9, 10*
Phorate	298-02-2	**X**	**X**	9
Phosphorus	7723-14-0		**X**	3, 9
Potassium	7440-09-7			3, 9, 10
Propionic acid	79-09-4	**X**		10
Propylbenzene	103-65-1	**X**		9
Pyrene	129-00-0	**X**	**X**	9, 10
Pyridine	110-86-1	**X**	**X**	3, 9, 10
Radium	7440-14-4			3
Radium-226	13982-63-3			3, 10
Radium-228	15262-20-1			3, 10
Safrole	94-59-7	**X**	**X**	3, 9
sec-Butylbenzene	135-98-8	**X**		9
Selenium	7782-49-2		**X**	3, 9, 10
Silica	*7631-86-9*			*10*
Silicon	7440-21-3			10
Silver	7440-22-4		**X**	3, 9, 10
Sodium	7440-23-5			3, 9, 10
Strontium	7440-24-6		**X**	3, 9, 10
Sulfate	*14808-79-8*			*3, 9, 10*
Sulfite	14265-45-3			3
Tetrachloroethylene	127-18-4	**X**	**X**	3, 9
Thallium	7440-28-0			3, 9, 10
Tin	7440-31-5		**X**	9, 10
Titanium	7440-32-6			3, 9, 10
Toluene	*108-88-3*	***X***	***X***	*3, 9, 10*
Vanadium	7440-62-2		**X**	3, 10

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Xylenes	*1330-20-7*	***X***	***X***	*3, 9, 10*
Zinc	*7440-66-6*		**X**	*3, 9, 10*
Zirconium	7440-67-7			3

A.2. References for Appendix A

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Appendix B

Water Acquisition Tables

Appendix B. Water Acquisition Tables

B.1. Supplemental Tables

Table B-1. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by state.

Hydraulic fracturing water use data from the EPA's project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c). Annual total water use data from the U.S. Geological Survey (USGS) Water Census (Maupin et al., 2014). Estimates of consumptions derived from hydraulic fracturing water use and total water use data. States listed in descending order by the volume of hydraulic fracturing water use.

State	Total annual water use in 2010 (millions of gal)[a,b]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[c]	Hydraulic fracturing water use compared to total water use (%)[d]	Hydraulic fracturing water consumption compared to total water consumption (%)[d,e]
Texas	9,052,000	19,942	0.2	0.7
Pennsylvania	2,967,450	5,105	0.2	1.4
Arkansas	4,124,500	3,676	0.1	0.1
Colorado	4,015,000	3,277	0.1	0.1
Oklahoma	1,157,050	2,949	0.3	0.8
Louisiana	3,117,100	2,462	0.1	0.4
North Dakota	419,750	2,181	0.5	2.9
West Virginia	1,288,450	657	0.1	0.5
Wyoming	1,715,500	538	<0.1	<0.1
New Mexico	1,153,400	371	<0.1	<0.1
Ohio	3,445,600	273	<0.1	0.1
Utah	1,627,900	251	<0.1	<0.1
Montana	2,792,250	155	<0.1	<0.1
Kansas	1,460,000	66	<0.1	<0.1
California	13,870,000	44	<0.1	<0.1
Michigan	3,942,000	28	<0.1	<0.1

State	Total annual water use in 2010 (millions of gal)[a,b]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[c]	Hydraulic fracturing water use compared to total water use (%)[d]	Hydraulic fracturing water consumption compared to total water consumption (%)[d,e]
Mississippi	1,434,450	18	<0.1	<0.1
Alaska[f]	397,850	7	<0.1	<0.1
Virginia	2,792,250	1	<0.1	<0.1
Alabama	3,635,400	1	<0.1	<0.1
TOTAL for all 20 states	64,407,900	42,001	0.1	0.2

[a] Texas, Colorado, Pennsylvania, North Dakota, Oklahoma, and Utah all made some degree of reporting to FracFocus mandatory rather than voluntary during this time period analyzed, January 1, 2011, to February 28, 2013. Three other states started requiring disclosure to either FracFocus or the state (Louisiana, Montana, and Ohio), and five states required or began requiring disclosure to the state (Arkansas, Michigan, New Mexico, West Virginia, and Wyoming). Alabama, Alaska, California, Kansas, Mississippi, and Virginia did not have reporting requirements during the period of time studied (U.S. EPA, 2015a).

[b] State-level data accessed from the USGS website (http://water.usgs.gov/watuse/data/2010/) on January 27, 2015. Total water withdrawals per day (located in downloaded Table 1) were multiplied by 365 days to estimate total water use for the year (Maupin et al., 2014).

[c] Average of water used for hydraulic fracturing in 2011 and 2012 as reported to FracFocus (U.S. EPA, 2015c).

[d] Percentages were calculated by averaging annual water use for hydraulic fracturing reported in FracFocus in 2011 and 2012 for a given state (U.S. EPA, 2015c), and then dividing by 2010 USGS hydraulic fracturing water use (Maupin et al., 2014) and multiplying by 100. Note that the annual hydraulic fracturing water use reported in FracFocus (the numerator) was not added to the 2010 total USGS water use value in the denominator, and the percentage is simply calculated as by dividing annual hydraulic fracturing use by 2010 total water use or consumption. This was done because of the difference in years between the two datasets, and because the USGS 2010 Census (Maupin et al., 2014) already included an estimate of hydraulic fracturing water use in its mining category. This approach is also consistent with that of other literature on this topic; see Nicot and Scanlon (2012).

[e] Consumption values were calculated with use-specific consumption rates predominantly from the USGS, including 19.2% for public supply, 19.2% for domestic use, 60.7% for irrigation, 60.7% for livestock, 14.8% for industrial uses, 14.8% for mining (Solley et al., 1998), and 2.7% for thermoelectric power (USGS, 2014). We used a rate of 71.6% for aquaculture (from Verdegem and Bosma, 2009) (evaporation per kg fish + infiltration per kg)/(total water use per kg) *100. These rates were multiplied by each USGS water use value (Maupin et al., 2014) to yield a total water consumption estimate. To calculate a consumption amount for hydraulic fracturing, we used a consumption rate of 82.5%. This was calculated by taking the median value for all reported produced water/injected water percentages in Tables 7-1 and 7-2 of this assessment and then subtracting from 100%. If a range of values was given, the midpoint was used. Note that this is likely a low estimate of consumption since much of this return water is not subsequently treated and reused, but rather disposed of in underground injection wells—see Chapter 8.

[f] All reported hydraulic fracturing disclosures for Alaska passed state locational quality assurance methods, but not county methods (U.S. EPA, 2015c). Thus, only state-level cumulative values were reported here, and no county-level data are provided in subsequent tables.

Table B-2. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by county.

Counties listed contained wells used for hydraulic fracturing according to the EPA's project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c). Annual total water use data from the USGS Water Census (Maupin et al., 2014). Estimates of consumption derived from hydraulic fracturing water use and total water use data.

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Alabama	Jefferson	29,685.5	0.6	<0.1	<0.1
	Tuscaloosa	14,319.0	0.5	<0.1	<0.1
Arkansas	Cleburne	9,471.8	740.9	7.8	32.9
	Conway	10,643.4	798.1	7.5	21.2
	Faulkner	3,204.7	284.0	8.9	13.7
	Independence	57,195.5	80.3	0.1	0.3
	Logan	1,525.7	2.4	0.2	0.3
	Sebastian	1,365.1	0.6	<0.1	<0.1
	Van Buren	1,587.8	899.6	56.7	168.8
	White	32,131.0	869.8	2.7	4.7
	Yell	1,507.5	<0.1	<0.1	<0.1
California	Colusa	304,782.3	<0.1	<0.1	<0.1
	Glenn	221,420.0	<0.1	<0.1	<0.1
	Kern	788,359.9	41.7	<0.1	<0.1
	Los Angeles	1,118,363.7	0.2	<0.1	<0.1
	Sutter	263,511.8	0.2	<0.1	<0.1
	Ventura	262,610.2	1.8	<0.1	<0.1
Colorado	Adams	84,285.8	3.2	<0.1	<0.1
	Arapahoe	68,255.0	4.0	<0.1	<0.1
	Boulder	84,537.7	4.1	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Colorado, cont.	Broomfield	2,336.0	4.5	0.2	0.4
	Delta	131,221.2	0.5	<0.1	<0.1
	Dolores	2,040.4	0.1	<0.1	<0.1
	El Paso	42,380.2	<0.1	<0.1	<0.1
	Elbert	5,040.7	<0.1	<0.1	<0.1
	Fremont	53,366.7	0.6	<0.1	<0.1
	Garfield	95,436.6	1,804.2	1.9	2.7
	Jackson	126,968.9	1.0	<0.1	<0.1
	La Plata	122,873.6	3.5	<0.1	<0.1
	Larimer	150,690.3	5.4	<0.1	<0.1
	Las Animas	26,911.5	7.9	<0.1	<0.1
	Mesa	275,476.5	122.1	<0.1	0.1
	Moffat	62,093.8	14.5	<0.1	<0.1
	Morgan	67,901.0	3.9	<0.1	<0.1
	Phillips	21,509.5	0.2	<0.1	<0.1
	Rio Blanco	97,513.4	147.3	0.2	0.2
	Routt	74,460.0	0.1	<0.1	<0.1
	San Miguel	13,848.1	0.3	<0.1	<0.1
	Weld	168,677.5	1,149.4	0.7	1.0
	Yuma	80,595.7	0.4	<0.1	<0.1
Kansas	Barber	2,164.5	9.9	0.5	0.7
	Clark	1,898.0	0.8	<0.1	0.1
	Comanche	3,011.3	25.6	0.9	1.2
	Finney	102,685.5	2.4	<0.1	<0.1
	Grant	47,128.8	0.2	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Kansas, cont.	Gray	69,379.2	3.3	<0.1	<0.1
	Harper	1,357.8	17.3	1.3	2.0
	Haskell	72,496.3	0.1	<0.1	<0.1
	Hodgeman	8,460.7	2.7	<0.1	<0.1
	Kearny	64,134.2	<0.1	<0.1	<0.1
	Lane	5,628.3	0.8	<0.1	<0.1
	Meade	55,958.2	<0.1	<0.1	<0.1
	Morton	17,403.2	<0.1	<0.1	<0.1
	Ness	1,478.3	1.6	0.1	0.2
	Seward	57,443.7	<0.1	<0.1	<0.1
	Sheridan	26,393.2	0.7	<0.1	<0.1
	Stanton	41,420.2	<0.1	<0.1	<0.1
	Stevens	72,124.0	0.1	<0.1	<0.1
	Sumner	3,442.0	0.2	<0.1	<0.1
Louisiana	Allen	8,942.5	0.1	<0.1	<0.1
	Beauregard	10,161.6	2.3	<0.1	0.1
	Bienville	4,810.7	108.9	2.3	10.0
	Bossier	5,599.1	110.1	2.0	4.9
	Caddo	53,644.1	153.6	0.3	1.7
	Calcasieu	81,621.3	0.1	<0.1	<0.1
	Caldwell	1,398.0	<0.1	<0.1	<0.1
	Claiborne	952.7	3.8	0.4	1.1
	De Soto	13,373.6	1,085.9	8.1	47.4
	East Feliciana	1,350.5	3.7	0.3	0.7
	Jackson	1,456.4	<0.1	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Louisiana, cont.	Lincoln	3,000.3	3.3	0.1	0.3
	Natchitoches	12,530.5	12.7	0.1	0.2
	Rapides	199,976.2	1.7	<0.1	<0.1
	Red River	1,606.0	569.6	35.5	83.2
	Sabine	1,522.1	395.2	26.0	76.6
	Tangipahoa	7,329.2	1.9	<0.1	0.1
	Union	1,481.9	4.9	0.3	1.0
	Webster	2,664.5	1.2	<0.1	0.1
	West Feliciana	15,191.3	2.3	<0.1	0.1
	Winn	846.8	1.1	0.1	0.4
Michigan	Cheboygan	2,777.7	<0.1	<0.1	<0.1
	Gladwin	850.5	1.1	0.1	0.4
	Kalkaska	1,233.7	24.0	1.9	3.7
	Missaukee	1,423.5	<0.1	<0.1	<0.1
	Ogemaw	1,179.0	<0.1	<0.1	<0.1
	Roscommon	1,000.1	2.4	0.2	0.9
Mississippi	Amite	792.1	14.4	1.8	3.8
	Wilkinson	1,270.2	3.2	0.3	0.4
Montana	Daniels	1,408.9	0.6	<0.1	0.1
	Garfield	1,631.6	0.5	<0.1	<0.1
	Glacier	46,760.2	5.1	<0.1	<0.1
	Musselshell	26,827.5	0.4	<0.1	<0.1
	Richland	94,797.8	83.5	0.1	0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Montana, cont.	Roosevelt	31,539.7	52.1	0.2	0.2
	Rosebud	71,412.3	3.5	<0.1	<0.1
	Sheridan	7,354.8	9.7	0.1	0.2
New Mexico	Chaves	88,078.2	2.8	<0.1	<0.1
	Colfax	17,450.7	0.7	<0.1	<0.1
	Eddy	70,612.9	225.6	0.3	0.5
	Harding	1,168.0	0.1	<0.1	<0.1
	Lea	64,057.5	113.7	0.2	0.3
	Rio Arriba	39,080.6	16.5	<0.1	0.1
	Roosevelt	63,367.7	<0.1	<0.1	<0.1
	San Juan	125,432.3	11.6	<0.1	<0.1
	Sandoval	23,922.1	0.4	<0.1	<0.1
North Dakota	Billings	762.9	44.4	5.8	16.2
	Bottineau	1,164.4	0.1	<0.1	<0.1
	Burke	394.2	63.6	16.1	40.8
	Divide	806.7	102.2	12.7	18.6
	Dunn	1,076.8	309.5	28.7	43.1
	Golden Valley	208.1	4.6	2.2	3.8
	Mckenzie	13,753.2	588.4	4.3	6.2
	Mclean	7,873.1	12.2	0.2	0.4
	Mountrail	1,248.3	449.4	36.0	98.3
	Stark	1,168.0	48.0	4.1	8.5
	Williams	7,705.2	558.5	7.2	11.3

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Ohio	Ashland	2,033.1	1.5	0.1	0.2
	Belmont	65,528.5	1.9	<0.1	0.1
	Carroll	1,127.9	152.7	13.5	37.3
	Columbiana	3,763.2	30.7	0.8	2.2
	Coshocton	53,775.5	5.4	<0.1	0.1
	Guernsey	2,379.8	8.4	0.4	0.7
	Harrison	481.8	16.5	3.4	7.3
	Jefferson	632,917.3	26.2	<0.1	0.1
	Knox	3,270.4	1.1	<0.1	0.1
	Medina	3,540.5	1.3	<0.1	0.1
	Muskingum	6,018.9	5.1	0.1	0.3
	Noble	478.2	8.3	1.7	3.4
	Portage	18,414.3	3.2	<0.1	0.1
	Stark	16,479.8	2.4	<0.1	<0.1
	Tuscarawas	14,165.7	6.7	<0.1	0.2
	Wayne	6,051.7	1.7	<0.1	0.1
Oklahoma	Alfalfa	2,996.7	182.7	6.1	12.0
	Beaver	15,341.0	23.1	0.2	0.3
	Beckham	4,099.0	108.0	2.6	4.7
	Blaine	3,763.2	203.3	5.4	9.3
	Bryan	5,062.6	10.3	0.2	0.4
	Caddo	24,064.5	25.4	0.1	0.3
	Canadian	5,584.5	441.9	7.9	15.6
	Carter	159,906.5	161.9	0.1	0.5
	Coal	1,193.6	85.9	7.2	21.5

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Oklahoma, cont.	Custer	3,281.4	19.0	0.6	1.2
	Dewey	10,953.7	162.6	1.5	6.2
	Ellis	8,486.3	184.3	2.2	3.2
	Garvin	16,279.0	15.0	0.1	0.4
	Grady	13,537.9	111.5	0.8	2.3
	Grant	5,569.9	77.8	1.4	5.2
	Harper	3,266.8	8.8	0.3	0.4
	Hughes	3,394.5	30.5	0.9	2.2
	Jefferson	4,496.8	<0.1	<0.1	<0.1
	Johnston	1,671.7	32.9	2.0	4.7
	Kay	16,957.9	17.3	0.1	0.4
	Kingfisher	3,744.9	10.2	0.3	0.5
	Kiowa	5,022.4	0.1	<0.1	<0.1
	Latimer	1,062.2	0.6	0.1	0.1
	Le Flore	8,635.9	0.3	<0.1	<0.1
	Logan	4,077.1	4.2	0.1	0.3
	Love	2,011.2	4.4	0.2	0.5
	Major	6,321.8	1.2	<0.1	<0.1
	Marshall	2,613.4	98.4	3.8	7.2
	McClain	2,952.9	2.1	0.1	0.2
	Noble	12,990.4	25.3	0.2	1.8
	Oklahoma	47,836.9	1.2	<0.1	<0.1
	Osage	6,971.5	3.8	0.1	0.2
	Pawnee	4,839.9	15.7	0.3	1.4
	Payne	4,332.6	9.9	0.2	0.6

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Oklahoma, cont.	Pittsburg	6,314.5	349.0	5.5	16.0
	Roger Mills	2,847.0	235.5	8.3	12.6
	Seminole	124,837.3	0.1	<0.1	<0.1
	Stephens	49,990.4	27.7	0.1	0.3
	Texas	110,208.1	0.1	<0.1	<0.1
	Washita	3,310.6	102.1	3.1	5.4
	Woods	4,139.1	155.1	3.7	10.9
Pennsylvania	Allegheny	234,140.2	13.6	<0.1	<0.1
	Armstrong	65,853.3	55.7	0.1	1.8
	Beaver	157,793.2	30.5	<0.1	0.2
	Blair	8,303.8	5.9	0.1	0.2
	Bradford	4,354.5	1,059.4	24.3	78.2
	Butler	5,730.5	121.8	2.1	6.0
	Cameron	292.0	6.6	2.3	4.1
	Centre	16,560.1	38.5	0.2	0.5
	Clarion	1,843.3	8.1	0.4	1.4
	Clearfield	111,051.3	111.5	0.1	2.3
	Clinton	6,161.2	94.4	1.5	3.0
	Columbia	3,810.6	5.6	0.1	0.4
	Crawford	5,091.8	2.4	<0.1	0.1
	Elk	7,876.7	37.5	0.5	1.9
	Fayette	16,465.2	120.2	0.7	2.7
	Forest	744.6	7.7	1.0	1.6
	Greene	13,023.2	359.0	2.8	24.7
	Huntingdon	5,121.0	2.7	0.1	0.2

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Pennsylvania, cont.	Indiana	21,819.7	16.2	0.1	0.7
	Jefferson	1,730.1	13.8	0.8	1.7
	Lawrence	36,598.6	27.0	0.1	1.0
	Lycoming	5,854.6	704.6	12.0	33.8
	McKean	4,723.1	60.5	1.3	4.9
	Potter	2,281.3	16.5	0.7	1.0
	Somerset	10,833.2	5.8	0.1	0.2
	Sullivan	222.7	66.5	29.9	79.8
	Susquehanna	1,617.0	751.3	46.5	123.4
	Tioga	2,909.1	566.3	19.5	47.3
	Venango	2,989.4	2.4	0.1	0.3
	Warren	5,099.1	2.3	<0.1	0.2
	Washington	130,535.0	433.7	0.3	4.6
	Westmoreland	14,607.3	207.0	1.4	3.8
	Wyoming	4,788.8	150.0	3.1	15.2
Texas	Andrews	23,363.7	236.2	1.0	2.7
	Angelina	5,540.7	0.8	<0.1	<0.1
	Archer	2,536.8	0.1	<0.1	<0.1
	Atascosa	15,038.0	327.3	2.2	4.0
	Austin	2,555.0	2.1	0.1	0.1
	Bee	3,087.9	20.0	0.6	1.1
	Borden	2,427.3	8.0	0.3	1.0
	Bosque	3,544.2	0.7	<0.1	<0.1
	Brazos	24,790.8	7.7	<0.1	0.1
	Brooks	1,204.5	1.5	0.1	0.3

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Burleson	10,694.5	3.0	<0.1	<0.1
	Cherokee	24,845.6	0.5	<0.1	<0.1
	Clay	1,963.7	<0.1	<0.1	<0.1
	Cochran	24,035.3	3.0	<0.1	<0.1
	Coke	12,713.0	0.3	<0.1	<0.1
	Colorado	52,465.1	0.1	<0.1	<0.1
	Concho	2,832.4	<0.1	<0.1	<0.1
	Cooke	4,533.3	454.3	10.0	29.9
	Cottle	733.7	0.3	<0.1	0.1
	Crane	8,566.6	92.3	1.1	5.7
	Crockett	4,281.5	279.0	6.5	29.5
	Crosby	27,261.9	1.3	<0.1	<0.1
	Culberson	14,311.7	37.7	0.3	0.4
	Dallas	112,204.7	5.6	<0.1	<0.1
	Dawson	28,842.3	17.5	0.1	0.1
	DeWitt	2,394.4	546.6	22.8	48.6
	Denton	60,684.9	455.0	0.7	2.3
	Dimmit	4,073.4	1,794.2	44.0	81.3
	Ector	21,958.4	226.5	1.0	4.6
	Edwards	332.2	<0.1	<0.1	<0.1
	Ellis	8,530.1	4.2	<0.1	0.1
	Erath	5,876.5	0.8	<0.1	<0.1
	Fayette	9,008.2	13.7	0.2	1.2
	Fisher	2,854.3	1.8	0.1	0.1
	Franklin	1,956.4	<0.1	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Freestone	297,861.9	53.9	<0.1	0.5
	Frio	20,589.7	127.5	0.6	0.9
	Gaines	121,778.6	21.6	<0.1	<0.1
	Garza	5,234.1	0.6	<0.1	<0.1
	Glasscock	20,680.9	598.1	2.9	4.2
	Goliad	142,963.2	<0.1	<0.1	<0.1
	Gonzales	7,121.2	577.9	8.1	17.6
	Grayson	8,143.2	9.3	0.1	0.3
	Gregg	33,010.6	9.4	<0.1	0.2
	Grimes	112,500.3	15.5	<0.1	0.3
	Hansford	43,643.1	2.9	<0.1	<0.1
	Hardeman	2,230.2	0.4	<0.1	<0.1
	Hardin	2,376.2	0.1	<0.1	<0.1
	Harrison	11,869.8	141.6	1.2	6.0
	Hartley	113,555.2	1.9	<0.1	<0.1
	Haskell	12,143.6	0.1	<0.1	<0.1
	Hemphill	3,150.0	263.9	8.4	16.3
	Hidalgo	171,630.3	8.0	<0.1	<0.1
	Hockley	46,314.9	3.0	<0.1	<0.1
	Hood	9,351.3	76.0	0.8	2.2
	Houston	3,686.5	8.6	0.2	0.6
	Howard	10,811.3	97.6	0.9	2.7
	Hutchinson	34,437.8	0.3	<0.1	<0.1
	Irion	1,335.9	411.4	30.8	74.5
	Jack	2,241.1	14.0	0.6	2.2

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Jefferson	88,585.5	<0.1	<0.1	<0.1
	Jim Hogg	306.6	0.1	<0.1	0.1
	Johnson	9,241.8	582.0	6.3	18.5
	Jones	5,679.4	<0.1	<0.1	<0.1
	Karnes	1,861.5	1,055.2	56.7	120.1
	Kenedy	456.3	0.2	0.1	0.1
	Kent	6,132.0	0.4	<0.1	<0.1
	King	1,485.6	<0.1	<0.1	<0.1
	Kleberg	1,171.7	3.4	0.3	0.5
	Knox	9,800.3	<0.1	<0.1	<0.1
	La Salle	2,474.7	1,288.7	52.1	93.7
	Lavaca	3,763.2	45.0	1.2	2.0
	Lee	3,120.8	1.2	<0.1	0.1
	Leon	2,171.8	56.2	2.6	6.6
	Liberty	20,662.7	<0.1	<0.1	<0.1
	Limestone	11,158.1	10.7	0.1	0.9
	Lipscomb	11,015.7	89.0	0.8	1.1
	Live Oak	1,916.3	294.0	15.3	40.1
	Loving	781.1	138.4	17.7	94.1
	Lynn	19,892.5	1.1	<0.1	<0.1
	Madison	1,554.9	45.3	2.9	8.2
	Marion	3,606.2	5.9	0.2	0.9
	Martin	14,063.5	432.0	3.1	4.7
	Maverick	20,498.4	52.4	0.3	0.4
	McMullen	657.0	745.9	113.5	350.4

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Medina	19,228.2	0.2	<0.1	<0.1
	Menard	1,014.7	<0.1	<0.1	<0.1
	Midland	12,891.8	307.4	2.4	3.7
	Milam	16,665.9	4.9	<0.1	0.1
	Mitchell	6,559.1	11.0	0.2	0.3
	Montague	3,989.5	925.3	23.2	77.8
	Montgomery	32,565.3	0.2	<0.1	<0.1
	Moore	57,075.1	<0.1	<0.1	<0.1
	Nacogdoches	5,891.1	271.7	4.6	12.5
	Navarro	18,699.0	4.8	<0.1	0.1
	Newton	2,263.0	0.2	<0.1	<0.1
	Nolan	4,124.5	4.5	0.1	0.2
	Nueces	85,767.7	1.0	<0.1	<0.1
	Ochiltree	21,348.9	33.3	0.2	0.2
	Oldham	2,124.3	1.3	0.1	0.1
	Orange	150,128.2	0.3	<0.1	<0.1
	Palo Pinto	18,403.3	9.6	0.1	0.3
	Panola	6,365.6	346.5	5.4	20.7
	Parker	8,241.7	261.7	3.2	9.8
	Pecos	52,954.2	8.2	<0.1	<0.1
	Polk	204,009.5	0.2	<0.1	<0.1
	Potter	2,029.4	0.4	<0.1	<0.1
	Reagan	9,333.1	410.5	4.4	7.8
	Reeves	20,772.2	164.2	0.8	1.1
	Roberts	7,690.6	38.2	0.5	1.2

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Robertson	158,344.3	45.4	<0.1	0.2
	Runnels	2,847.0	<0.1	<0.1	<0.1
	Rusk	582,134.9	65.8	<0.1	0.3
	Sabine	799.4	31.1	3.9	13.9
	San Augustine	1,131.5	182.1	16.1	50.8
	San Patricio	4,172.0	1.1	<0.1	<0.1
	Schleicher	967.3	27.0	2.8	5.0
	Scurry	14,187.6	1.1	<0.1	<0.1
	Shelby	4,920.2	133.6	2.7	8.2
	Sherman	78,073.5	<0.1	<0.1	<0.1
	Smith	11,231.1	0.2	<0.1	<0.1
	Somervell	746,005.3	4.8	<0.1	<0.1
	Starr	9,552.1	5.0	0.1	0.1
	Stephens	13,446.6	2.6	<0.1	0.1
	Sterling	719.1	36.6	5.1	11.9
	Stonewall	923.5	0.9	0.1	0.3
	Sutton	1,153.4	1.6	0.1	0.3
	Tarrant	104,430.2	1,443.0	1.4	3.9
	Terrell	543.9	0.1	<0.1	<0.1
	Terry	48,362.5	7.5	<0.1	<0.1
	Tyler	1,872.5	0.1	<0.1	<0.1
	Upshur	8,610.4	0.2	<0.1	<0.1
	Upton	7,975.3	462.6	5.8	14.2
	Van Zandt	4,139.1	0.1	<0.1	<0.1
	Walker	4,478.6	3.4	0.1	0.2

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Texas, cont.	Waller	9,829.5	0.1	<0.1	<0.1
	Ward	6,909.5	107.3	1.6	4.6
	Washington	2,430.9	2.2	0.1	0.2
	Webb	15,862.9	1,117.8	7.0	18.2
	Wharton	81,606.7	<0.1	<0.1	<0.1
	Wheeler	6,522.6	858.0	13.2	21.5
	Wichita	25,936.9	0.1	<0.1	<0.1
	Wilbarger	12,683.8	0.2	<0.1	<0.1
	Willacy	15,209.6	0.1	<0.1	<0.1
	Wilson	7,843.9	84.5	1.1	1.7
	Winkler	5,274.3	7.7	0.1	0.5
	Wise	24,966.0	529.7	2.1	8.9
	Wood	19,334.1	0.2	<0.1	<0.1
	Yoakum	77,325.3	7.5	<0.1	<0.1
	Young	21,162.7	0.1	<0.1	<0.1
	Zapata	2,697.4	1.1	<0.1	0.1
	Zavala	14,410.2	130.0	0.9	1.3
Utah	Carbon	15,067.2	7.3	<0.1	0.1
	Duchesne	119,811.3	85.5	0.1	0.1
	San Juan	10,632.5	0.3	<0.1	<0.1
	Sevier	52,512.6	<0.1	<0.1	<0.1
	Uintah	100,229.0	157.5	0.2	0.2
Virginia	Buchanan	313.9	0.6	0.2	0.3
	Dickenson	1,741.1	0.8	<0.1	0.2
	Wise	1,927.2	0.1	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
West Virginia	Barbour	773.8	19.9	2.6	6.9
	Brooke	4,551.6	54.8	1.2	5.1
	Doddridge	405.2	78.5	19.4	69.4
	Hancock	28,718.2	1.2	<0.1	<0.1
	Harrison	20,232.0	40.2	0.2	1.9
	Lewis	901.6	2.4	0.3	0.8
	Marion	5,982.4	70.1	1.2	4.9
	Marshall	158,358.9	84.5	0.1	0.7
	Monongalia	42,102.8	6.8	<0.1	0.1
	Ohio	3,825.2	116.5	3.0	10.4
	Pleasants	24,703.2	<0.1	<0.1	<0.1
	Preston	2,890.8	8.4	0.3	1.4
	Ritchie	587.7	2.8	0.5	1.7
	Taylor	824.9	52.9	6.4	17.6
	Tyler	4,934.8	2.1	<0.1	0.2
	Upshur	1,814.1	34.9	1.9	6.8
	Webster	1,292.1	2.3	0.2	0.3
	Wetzel	1,467.3	78.2	5.3	11.9
Wyoming	Big Horn	143,368.4	2.9	<0.1	<0.1
	Campbell	44,318.3	11.7	<0.1	0.1
	Carbon	137,130.5	4.5	<0.1	<0.1
	Converse	56,972.9	106.8	0.2	0.3
	Fremont	186,150.0	28.2	<0.1	<0.1
	Goshen	144,248.0	5.8	<0.1	<0.1
	Hot Springs	28,572.2	0.3	<0.1	<0.1

State	County	Total annual water use in 2010 (millions of gal)[a]	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal)[b]	Hydraulic fracturing water use compared to total water use (%)[c]	Hydraulic fracturing water consumption compared to total water consumption (%)[c,d]
Wyoming, cont.	Johnson	43,205.1	<0.1	<0.1	<0.1
	Laramie	86,297.0	18.3	<0.1	<0.1
	Lincoln	74,562.2	0.8	<0.1	<0.1
	Natrona	62,885.9	1.8	<0.1	<0.1
	Niobrara	25,148.5	0.1	<0.1	<0.1
	Park	111,317.7	0.9	<0.1	<0.1
	Sublette	61,006.1	314.8	0.5	0.7
	Sweetwater	61,699.6	39.4	0.1	0.1
	Uinta	79,518.9	0.6	<0.1	<0.1
	Washakie	60,400.2	1.1	<0.1	<0.1

[a] County-level data accessed from the USGS website (http://water.usgs.gov/watuse/data/2010/) on November 11, 2014. Total daily water withdrawals were multiplied by 365 days to estimate total water use for the year (Maupin et al., 2014).

[b] Average of water used for hydraulic fracturing in 2011 and 2012, as reported to FracFocus (U.S. EPA, 2015c).

[c] Percentages were calculated by averaging annual water use for hydraulic fracturing reported in FracFocus in 2011 and 2012 for a given county (U.S. EPA, 2015c), and then dividing by 2010 USGS total water use for that county (Maupin et al., 2014) and multiplying by 100.

[d] Consumption values were calculated with use-specific consumption rates predominantly from the USGS, including 19.2% for public supply, 19.2% for domestic use, 60.7% for irrigation, 60.7% for livestock, 14.8% for industrial uses, 14.8% for mining (Solley et al., 1998), and 2.7% for thermoelectric power (USGS, 2014). We used a rate of 71.6% for aquaculture (from Verdegem and Bosma, 2009) (evaporation per kg fish + infiltration per kg)/(total water use per kg)*100. These rates were multiplied by each USGS water use value (Maupin et al., 2014) to yield a total water consumption estimate. To calculate a consumption amount for hydraulic fracturing, we used a consumption rate of 82.5%. This was calculated by taking the median value for all reported produced water/injected water percentages in Tables 7-1 and 7-2 of this assessment and then subtracting from 100%. If a range of values was given, the midpoint was used. Note that this is likely a low estimate of consumption since much of this return water is not subsequently treated and reused, but rather disposed of in underground injection wells—see Chapter 8.

Table B-3. Comparison of water use per well estimates from the EPA's project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and literature sources.

Source: (U.S. EPA, 2015c)

State	Basin[a]	Water use per well (gal) - FracFocus estimate[b]	Water use per well (gal) - Literature estimate[b,c]	FracFocus estimate as a percentage of literature estimate (%)
Colorado	Denver	403,686	2,900,000	14
North Dakota		2,140,842	2,200,000	97
Oklahoma		2,591,778	3,000,000	86
Pennsylvania[d]		4,301,701	4,450,000	97
Texas	Fort Worth	3,881,220	4,500,000	86
Texas	Salt	3,139,980	4,000,000	78
Texas	Western Gulf	3,777,648	4,600,000	82
Average[e]				77
Median[e]				86

[a] In cases where a basin is not specified, estimates were for the entire state and not specific to a particular basin. Basin boundaries for the FracFocus estimates were determined from data from the U.S. EIA (see U.S. EPA, 2015b).

[b] The type of literature estimate determined the specific comparison with FracFocus. If averages were given in the literature (as for North Dakota and Pennsylvania), those values were compared with FracFocus averages; where medians were given in the literature (as for Colorado, Oklahoma, and Texas), they were compared with FracFocus medians.

[c] Literature estimates were from the following sources: Colorado (Goodwin et al., 2014), North Dakota (North Dakota State Water Commission, 2014), Pennsylvania (Mitchell et al., 2013), and Texas (Nicot et al., 2012)—see far right-column and footnotes in Table B-5 for details on literature estimates. Where the literature provided a range, the mid-point was used. Only literature estimates that were not directly derived from FracFocus were included.

[d] The results from Mitchell et al. (2013) were used for Pennsylvania since they were derived from Pennsylvania Department of Environment Protection records. Estimates from Hansen et al. (2013) were not included here because they were based on FracFocus.

[e] Average and median percentage calculations were not weighted by the number of wells for a given estimate.

Table B-4. Comparison of well counts from the EPA's project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and state databases for North Dakota, Pennsylvania, and West Virginia.

State	FracFocus well counts[a]			State database well counts			FracFocus counts as a percentage of state database counts		
	2011	2012	Total	2011	2012	Total	2011	2012	Total
North Dakota[b]	613	1,458	2,071	1,225	1,740	2,965	50%	84%	70%
Pennsylvania[c]	1,137	1,257	2,394	1,963	1,347	3,310	58%	93%	72%
West Virginia[d]	93	176	269	214	251	465	43%	70%	58%
Average							50%	82%	67%

[a] FracFocus disclosures from U.S. EPA (2015c).

[b] For North Dakota state well counts, we used a North Dakota Department of Mineral Resources online database containing a list of horizontal wells completed in the Bakken Formation. Data for North Dakota were accessed on July 9, 2014 at https://www.dmr.nd.gov/oilgas/bakkenwells.asp.

[c] For Pennsylvania state well counts, we used completed horizontal wells as a proxy for hydraulically fractured wells in the state. The Pennsylvania Department of Environmental Protection has online databases of permitted and spudded wells, which differentiate between conventional and unconventional wells and can generate summary statistics at both the county and state scale. The number of spudded wells (i.e., wells drilled) provided a better comparison with the number of hydraulically fractured wells in FracFocus than that of permitted wells. The number of permitted wells was nearly double that of spudded in 2011 and 2012, indicating that almost half of the wells permitted were not drilled in that same year. Therefore, we used spudded wells here. Data for Pennsylvania were accessed on February 11, 2014 from http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?/Oil_Gas/Spud_External_Data.

[d] For West Virginia state well counts, data on the number of hydraulically fractured wells per year were received from the West Virginia Department of Environmental Protection on February 25, 2014.

Table B-5. Water use per hydraulically fractured well as reported in the EPA's project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) by state and basin.

Souce: (U.S. EPA, 2015c)
Other literature estimates are also included where available. NA indicates other literature estimates were not available. All FracFocus estimates were limited to disclosures with valid state, county, and volume information. States listed in order addressed in Chapter 4.

State	Basin/total[a]	Number of disclosures	Mean (gal)	Median (gal)	10th percentile (gal)	90th percentile (gal)	Literature estimates
Texas	Permian	8,419	1,068,511	841,134	40,090	1,814,633	Many formations reported[b]
	Western Gulf	4,549	3,915,540	3,777,648	173,832	6,786,052	4.5–4.7 million gal (median, Eagle Ford play)[b]
	Fort Worth	2,564	3,880,724	3,881,220	923,381	6,649,406	4.5 million gal (median, Barnett play)[b]
	TX-LA-MS Salt	626	4,261,363	3,139,980	193,768	10,010,707	6–7.5 million gal (median, Texas-Haynesville play) and 0.5-1 million gallons (median, Cotton Valley play)[b]
	Anadarko	604	4,128,702	3,341,310	492,421	8,292,996	Many formations reported[b]
	Other	120	1,601,897	184,239	21,470	5,678,588	NA
	Total	16,882	2,494,452	1,420,613	58,709	6,115,195	Not reported by state[b]
Colorado	Denver	3,166	753,887	403,686	143,715	2,588,946	2.9 million gal (median, Wattenberg field of Niobrara play)[c]
	Uinta-Piceance	1,520	2,739,523	1,798,414	840,778	5,066,380	NA
	Raton	146	108,003	95,974	24,917	211,526	NA
	Other	66	605,740	183,408	34,412	601,816	NA
	Total	4,898	1,348,842	463,462	147,353	3,092,024	NA

State	Basin/total[a]	Number of disclosures	Mean (gal)	Median (gal)	10th percentile (gal)	90th percentile (gal)	Literature estimates
Wyoming	Greater Green River	861	841,702	752,979	147,020	1,493,266	NA
	Powder River	351	739,129	5,927	5,353	2,863,182	NA
	Other	193	613,618	41,664	22,105	1,818,606	NA
	Total	1,405	784,746	322,793	5,727	1,837,602	NA
Pennsylvania	Appalachian	2,445	4,301,701	4,184,936	2,313,649	6,615,981	4.2-4.6 million gal (average, Marcellus play, Susquehanna River Basin)[d]
	Total	2,445	4,301,701	4,184,936	2,313,649	6,615,981	4.1-4.5[d] and 4.3-4.6[e] million gal (average)
West Virginia	Appalachian	273	5,034,217	5,012,238	3,170,210	7,297,080	NA
	Total	273	5,034,217	5,012,238	3,170,210	7,297,080	4.7-6 million gal (average)[d]
Ohio	Appalachian	146	4,206,955	3,887,499	2,885,568	5,571,027	NA
	Total	146	4,206,955	3,887,499	2,885,568	5,571,027	NA
North Dakota	Williston	2,109	2,140,842	2,022,380	969,380	3,313,482	NA
	Total	2,109	2,140,842	2,022,380	969,380	3,313,482	2.2 million gal (average)[f]
Montana	Williston	187	1,640,085	1,552,596	375,864	3,037,398	NA
	Other	20	945,541	1,017,701	157,639	1,575,197	NA
	Total	207	1,572,979	1,455,757	367,326	2,997,552	NA
Oklahoma	Anadarko	935	3,742,703	3,259,774	1,211,700	6,972,652	Many formations reported[g]
	Arkoma	158	6,323,750	6,655,929	172,375	9,589,554	Many formations reported[g]
	Ardmore	98	6,637,332	8,021,559	81,894	8,835,842	Many formations reported[g]
	Other	592	1,963,480	1,866,144	1,319,247	2,785,352	NA
	Total	1,783	3,539,775	2,591,778	1,260,906	7,402,230	3 million gal (median)[g]

State	Basin/total[a]	Number of disclosures	Mean (gal)	Median (gal)	10th percentile (gal)	90th percentile (gal)	Literature estimates
Kansas	Total	121	1,135,973	1,453,788	10,836	2,227,926	NA
Arkansas	Arkoma	1,423	5,190,254	5,259,965	3,234,963	7,121,249	NA
	Total	1,423	5,190,254	5,259,965	3,234,963	7,121,249	NA
Louisiana	TX-LA-MS Salt	939	5,289,100	5,116,650	2,851,654	7,984,838	NA
	Other	27	896,899	232,464	87,003	3,562,400	NA
	Total	966	5,166,337	5,077,863	1,812,099	7,945,630	NA
Utah	Uinta-Piceance	1,396	375,852	304,105	77,166	770,699	NA
	Other	10	58,874	56,245	28,745	97,871	NA
	Total	1,406	373,597	302,075	76,286	769,360	NA
New Mexico	Permian	732	991,369	426,258	89,895	2,502,923	NA
	San Juan	363	159,680	97,734	27,217	313,919	NA
	Other	50	33,787	8,358	1,100	98,841	NA
	Total	1,145	685,882	175,241	35,638	1,871,666	NA

State	Basin/total[a]	Number of disclosures	Mean (gal)	Median (gal)	10th percentile (gal)	90th percentile (gal)	Literature estimates
California	San Joaquin	677	131,653	77,238	22,100	285,029	NA
	Other	34	132,391	36,099	13,768	361,192	NA
	Total	711	131,689	76,818	21,462	285,306	130,000 gallon (average)[h]

[a] Basin boundaries for the FracFocus estimates were determined from data from the U.S. EIA (see U.S. EPA, 2015b).

[b] Literature estimates for Texas were from Nicot et al. (2012), using proprietary data from IHS. In most cases, Nicot et al. reported at the play scale or smaller, rather than the EIA basin scale used for FracFocus. We reference 2011 and 2012 (partial year) for Nicot et al. where possible to overlap with the period of study for FracFocus, though more years were available for most formations. A range is reported for some medians because median water use was different for the two years. There were five formations reported for the Permian Basin (Wolfberry, Wolfcamp, Canyon, Clearfork, and San Andres-Greyburg). The most active area in the Permian Basin in 2011–2012 was the Wolfberry, which reported a median of 1 to 1.1 million gallons per well—these were mostly vertical wells. For the TX-LA-MS Salt Basin, Nicot et al. reported two formations (TX-Haynesville and Cotton Valley), with similar levels of activity in 2011-2012. Wells in TX-Haynesville were predominantly horizontal, while those in Cotton Valley were predominantly vertical (though horizontal wells in Cotton Valley were also reported). There were three fields reported in the Anadarko Basin (Granite Wash, Cleveland, and Marmaton). The most active area in the Anadarko Basin in 2011-2012 was the Granite Wash, which reported a median of 3.3 to 5.2 million gallons per well and where wells were mostly horizontal.

[c] Literature estimates for the Denver Basin were from Goodwin et al. (2014). Goodwin et al. assessed 200 randomly sampled wells in the Wattenberg Field of the Denver Basin (Niobrara Play), using industry data for wells operated by Noble Energy, drilled between January 1, 2010, and July 1, 2013. Water consumption is reported rather than water use, but Goodwin et al. assume, based on Noble Energy practices, that water use and water consumption were identical because none of the flowback or produced water is reused for hydraulic fracturing. Goodwin et al. reported drilling water consumed, hydraulic fracturing water consumed, and total water consumed. We present hydraulic fracturing water consumption here (hydraulic fracturing water consumption was approximately 95% of the total).

[d] Hansen et al. (2013), using data from FracFocus via Skytruth. For the Susquehanna River Basin portion of the Marcellus play, and for Pennsylvania as a whole, the range of annual averages is reported for 2011 and 2012. Similarly, for West Virginia, the range of annual averages is reported for 2011 and 2012 (partial year).

[e] Mitchell et al. (2013), using data reported to the Pennsylvania Department of Environmental Protection. Mitchell et al. reported water use in the Ohio River Basin for 2011 and 2012 (partial year) for horizontal and vertical wells. Here we report results for horizontal wells, which made up the majority of wells over the two-year period (i.e., 93%, 1,191 horizontal wells versus 96 vertical wells). A range is reported as before because the average water use differed between the two years.

[f] Literature estimates for North Dakota were from an informational bulletin from the North Dakota State Water Commission (2014). No further information was available.

[g] Murray (2013), who assessed water use for oil and gas operations from 2000–2010 for eight formations in Oklahoma using data from the Oklahoma Corporation Commission. It is not possible to extract an estimate corresponding to 2011–2012 from Murray without the raw data, because medians were presented for the 10-year period rather than separated by year.

[h] Literature estimates for California were from a California Council on Science and Technology report using data from FracFocus (CCST, 2014).

Table B-6. Estimated percent domestic use water from ground water and self-supplied by county.

Counties listed contained hydraulically fractured wells with valid state, county, and volume information (U.S. EPA, 2015c).
Data estimated from the USGS Water Census (Maupin et al., 2014).

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Alabama	Jefferson	11.9	0.8
	Tuscaloosa	10.7	6.1
Arkansas	Cleburne	0.0	0.0
	Conway	8.6	8.6
	Faulkner	48.0	3.5
	Independence	20.5	9.4
	Logan	0.0	0.0
	Sebastian	0.0	0.0
	Van Buren	6.4	6.4
	White	0.4	0.0
	Yell	1.8	1.8
California	Colusa	97.9	10.3
	Glenn	96.5	21.6
	Kern	74.5	1.7
	Los Angeles	45.0	4.2
	Sutter	19.4	4.6
	Ventura	30.9	3.9
Colorado	Adams	18.1	2.8
	Arapahoe	19.3	1.3
	Boulder	1.7	1.5
	Broomfield	0.0	0.0
	Delta	59.6	28.4
	Dolores	55.2	51.4
	El Paso	19.6	5.1
	Elbert	100.0	75.2
	Fremont	15.6	15.6

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Colorado, cont.	Garfield	36.7	28.5
	Jackson	84.4	40.7
	La Plata	24.4	11.3
	Larimer	2.3	0.8
	Las Animas	26.3	16.0
	Mesa	7.3	6.2
	Moffat	36.4	25.8
	Morgan	57.9	4.9
	Phillips	100.0	25.3
	Rio Blanco	60.2	32.5
	Routt	22.6	5.9
	San Miguel	71.4	32.5
	Weld	4.7	0.7
	Yuma	100.0	38.1
Kansas	Barber	100.0	19.0
	Clark	100.0	24.2
	Comanche	100.0	19.2
	Finney	100.0	2.1
	Grant	100.0	23.8
	Gray	100.0	36.4
	Harper	100.0	10.3
	Haskell	100.0	35.2
	Hodgeman	100.0	42.3
	Kearny	100.0	14.6
	Lane	100.0	24.1
	Meade	100.0	25.4
	Morton	100.0	21.7
	Ness	100.0	24.2
	Seward	100.0	15.7

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Kansas, cont.	Sheridan	100.0	44.9
	Stanton	100.0	29.8
	Stevens	100.0	25.9
	Sumner	51.3	0.0
Louisiana	Allen	100.0	7.5
	Beauregard	100.0	20.6
	Bienville	100.0	16.8
	Bossier	29.4	14.6
	Caddo	12.2	8.8
	Calcasieu	98.3	12.7
	Caldwell	100.0	6.5
	Claiborne	100.0	10.4
	De Soto	55.8	21.8
	East Feliciana	100.0	11.8
	Jackson	100.0	13.8
	Lincoln	100.0	4.2
	Natchitoches	23.2	11.4
	Rapides	100.0	3.3
	Red River	83.2	27.6
	Sabine	67.5	36.2
	Tangipahoa	100.0	26.9
	Union	100.0	11.2
	Webster	100.0	11.3
	West Feliciana	100.0	2.4
	Winn	100.0	16.4
Michigan	Cheboygan	100.0	76.4
	Gladwin	100.0	84.5
	Kalkaska	100.0	89.0
	Missaukee	100.0	90.6
	Ogemaw	100.0	90.8
	Roscommon	100.0	91.9

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Mississippi	Amite	100.0	26.0
	Wilkinson	100.0	11.1
Montana	Daniels	100.0	29.4
	Garfield	100.0	70.0
	Glacier	62.1	17.7
	Musselshell	89.9	54.5
	Richland	100.0	30.8
	Roosevelt	84.2	20.9
	Rosebud	51.3	10.3
	Sheridan	100.0	31.0
New Mexico	Chaves	100.0	11.8
	Colfax	30.7	2.6
	Eddy	100.0	2.2
	Harding	100.0	25.0
	Lea	100.0	17.4
	Rio Arriba	84.0	42.3
	Roosevelt	100.0	8.9
	San Juan	14.6	12.9
	Sandoval	98.9	23.2
North Dakota	Billings	NA	33.3
	Bottineau	100.0	13.7
	Burke	100.0	12.5
	Divide	100.0	12.5
	Dunn	100.0	21.4
	Golden Valley	100.0	7.7
	Mckenzie	75.8	15.7
	Mclean	12.5	9.9
	Mountrail	65.7	11.5
	Stark	NA	5.7
	Williams	27.4	7.3

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Ohio	Ashland	98.8	57.4
	Belmont	76.4	8.9
	Carroll	96.4	76.4
	Columbiana	63.2	43.2
	Coshocton	99.3	34.9
	Guernsey	37.6	9.5
	Harrison	65.6	45.9
	Jefferson	33.1	10.2
	Knox	99.2	41.1
	Medina	98.4	83.1
	Muskingum	93.4	17.0
	Noble	8.0	8.0
	Portage	32.6	18.3
	Stark	91.2	30.9
	Tuscarawas	94.0	23.5
	Wayne	99.1	49.0
Oklahoma	Alfalfa	100.0	14.6
	Beaver	100.0	47.9
	Beckham	100.0	10.6
	Blaine	100.0	8.8
	Bryan	26.0	7.8
	Caddo	45.4	35.1
	Canadian	100.0	0.0
	Carter	17.5	0.5
	Coal	31.5	27.5
	Custer	70.8	13.2
	Dewey	100.0	22.5
	Ellis	100.0	31.4
	Garvin	41.3	15.8
	Grady	100.0	34.2
	Grant	100.0	13.2
	Harper	100.0	22.6

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Oklahoma, cont.	Hughes	23.6	6.7
	Jefferson	13.5	1.8
	Johnston	53.4	1.1
	Kay	39.2	4.6
	Kingfisher	100.0	28.3
	Kiowa	10.3	0.0
	Latimer	12.6	12.6
	Le Flore	14.3	13.1
	Logan	61.1	34.6
	Love	100.0	3.8
	Major	100.0	28.1
	Marshall	20.1	4.4
	Mcclain	95.9	23.9
	Noble	23.3	14.3
	Oklahoma	22.0	2.5
	Osage	18.0	14.9
	Pawnee	38.2	27.7
	Payne	47.9	12.6
	Pittsburg	0.6	0.0
	Roger Mills	80.1	19.4
	Seminole	78.8	16.1
	Stephens	99.2	14.9
	Texas	100.0	10.9
	Washita	53.9	18.2
	Woods	100.0	14.7
Pennsylvania	Allegheny	15.7	15.3
	Armstrong	45.3	36.8
	Beaver	54.7	26.8
	Blair	34.9	24.0
	Bradford	100.0	65.2
	Butler	51.8	42.8
	Cameron	29.0	29.0

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Pennsylvania, cont.	Centre	93.1	21.3
	Clarion	61.5	55.8
	Clearfield	38.4	22.7
	Clinton	48.4	38.1
	Columbia	77.5	56.7
	Crawford	97.7	66.0
	Elk	25.3	15.6
	Fayette	19.2	16.1
	Forest	100.0	78.3
	Greene	31.9	31.9
	Huntingdon	73.2	57.8
	Indiana	52.2	49.1
	Jefferson	60.7	46.1
	Lawrence	40.5	38.8
	Lycoming	60.0	29.3
	McKean	56.6	33.3
	Potter	93.7	58.1
	Somerset	42.6	33.5
	Sullivan	100.0	76.9
	Susquehanna	79.9	74.7
	Tioga	81.3	58.3
	Venango	95.9	32.7
	Warren	96.9	49.4
	Washington	21.6	21.5
	Westmoreland	21.3	19.8
	Wyoming	100.0	70.6
Texas	Andrews	100.0	23.4
	Angelina	100.0	9.8
	Archer	16.9	16.9
	Atascosa	100.0	16.3
	Austin	100.0	55.6
	Bee	100.0	52.5

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Texas, cont.	Borden	100.0	71.4
	Bosque	88.7	30.3
	Brazos	100.0	2.1
	Brooks	100.0	35.3
	Burleson	100.0	42.9
	Cherokee	87.5	26.1
	Clay	44.6	36.7
	Cochran	100.0	23.3
	Coke	29.0	28.9
	Colorado	100.0	45.4
	Concho	96.8	5.0
	Cooke	75.5	8.9
	Cottle	100.0	21.4
	Crane	100.0	14.3
	Crockett	100.0	42.5
	Crosby	35.6	19.0
	Culberson	100.0	13.8
	Dallas	1.0	0.7
	Dawson	100.0	33.8
	DeWitt	100.0	42.3
	Denton	9.0	3.6
	Dimmit	100.0	30.5
	Ector	100.0	28.3
	Edwards	100.0	42.1
	Ellis	32.2	7.9
	Erath	100.0	43.3
	Fayette	100.0	27.6
	Fisher	NA	36.8
	Franklin	0.9	0.0
	Freestone	100.0	31.2
	Frio	100.0	20.4
	Gaines	100.0	45.5

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Texas, cont.	Garza	20.1	17.2
	Glasscock	NA	100.0
	Goliad	NA	66.7
	Gonzales	96.8	15.9
	Grayson	56.0	4.2
	Gregg	20.8	14.1
	Grimes	100.0	26.0
	Hansford	100.0	16.4
	Hardeman	87.6	13.3
	Hardin	100.0	29.5
	Harrison	43.8	24.8
	Hartley	100.0	39.7
	Haskell	100.0	15.7
	Hemphill	100.0	27.5
	Hidalgo	9.2	1.6
	Hockley	100.0	27.4
	Hood	70.8	39.8
	Houston	79.7	36.6
	Howard	100.0	19.8
	Hutchinson	27.3	14.9
	Irion	100.0	50.0
	Jack	46.7	43.8
	Jefferson	25.0	5.8
	Jim Hogg	NA	25.0
	Johnson	34.9	6.8
	Jones	60.5	60.5
	Karnes	100.0	17.6
	Kenedy	100.0	25.0
	Kent	100.0	37.5
	King	100.0	33.3
	Kleberg	100.0	1.9
	Knox	86.2	24.2

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Texas, cont.	La Salle	100.0	43.3
	Lavaca	100.0	56.0
	Lee	100.0	15.9
	Leon	100.0	41.4
	Liberty	98.5	42.5
	Limestone	46.5	32.5
	Lipscomb	100.0	23.5
	Live Oak	32.8	32.1
	Loving	NA	0.0
	Lynn	64.1	32.2
	Madison	100.0	66.9
	Marion	13.7	8.4
	Martin	100.0	48.9
	Maverick	27.6	27.6
	McMullen	100.0	40.0
	Medina	98.0	23.6
	Menard	36.4	36.4
	Midland	100.0	22.1
	Milam	82.5	41.1
	Mitchell	100.0	14.7
	Montague	57.1	49.7
	Montgomery	100.0	26.6
	Moore	100.0	8.1
	Nacogdoches	55.6	21.6
	Navarro	22.0	22.0
	Newton	100.0	63.7
	Nolan	100.0	17.6
	Nueces	5.6	5.6
	Ochiltree	100.0	16.8
	Oldham	100.0	58.8
	Orange	99.1	41.2
	Palo Pinto	11.7	11.7

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Texas, cont.	Panola	96.6	58.7
	Parker	63.5	41.1
	Pecos	100.0	31.3
	Polk	41.9	41.7
	Potter	100.0	12.6
	Reagan	100.0	16.2
	Reeves	100.0	31.1
	Roberts	100.0	33.3
	Robertson	97.1	22.5
	Runnels	13.5	13.5
	Rusk	90.7	41.8
	Sabine	76.2	69.0
	San Augustine	78.0	74.4
	San Patricio	88.8	21.8
	Schleicher	100.0	40.0
	Scurry	32.5	27.7
	Shelby	66.2	58.2
	Sherman	100.0	33.3
	Smith	48.0	13.7
	Somervell	87.7	69.3
	Starr	23.2	23.2
	Stephens	13.5	13.5
	Sterling	NA	18.8
	Stonewall	NA	40.0
	Sutton	100.0	26.7
	Tarrant	3.7	1.3
	Terrell	100.0	25.0
	Terry	100.0	16.7
	Tyler	100.0	73.6
	Upshur	54.1	23.2
	Upton	100.0	15.2
	Van Zandt	65.7	39.0

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Texas, cont.	Walker	57.7	30.6
	Waller	100.0	37.2
	Ward	100.0	4.5
	Washington	48.2	36.0
	Webb	99.4	0.5
	Wharton	100.0	45.9
	Wheeler	100.0	31.3
	Wichita	8.8	2.9
	Wilbarger	100.0	11.5
	Willacy	28.4	28.4
	Wilson	100.0	6.9
	Winkler	100.0	3.8
	Wise	51.3	50.4
	Wood	21.3	12.9
	Yoakum	100.0	36.0
	Young	19.3	18.9
	Zapata	13.9	13.9
	Zavala	100.0	15.2
Utah	Carbon	50.0	1.2
	Duchesne	57.1	10.4
	San Juan	68.3	47.5
	Sevier	100.0	10.0
	Uintah	87.7	3.1
Virginia	Buchanan	NA	27.6
	Dickenson	2.5	2.5
	Wise	5.9	2.3
West Virginia	Barbour	24.1	24.8
	Brooke	33.4	6.8
	Doddridge	60.6	62.1
	Hancock	67.7	6.9
	Harrison	8.8	8.9
	Lewis	29.5	30.3

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
West Virginia, cont.	Marion	5.8	4.9
	Marshall	96.5	12.0
	Monongalia	5.3	5.5
	Ohio	5.4	3.4
	Pleasants	100.0	27.9
	Preston	66.1	41.0
	Ritchie	45.2	46.4
	Taylor	14.9	14.9
	Tyler	44.4	39.2
	Upshur	27.3	27.8
	Webster	41.9	43.2
	Wetzel	96.3	28.6
Wyoming	Big Horn	79.4	11.3
	Campbell	100.0	0.6
	Carbon	63.8	6.7
	Converse	96.5	17.0
	Fremont	49.3	23.7
	Goshen	100.0	21.1
	Hot Springs	31.9	8.2
	Johnson	40.8	35.4
	Laramie	38.1	13.0
	Lincoln	82.4	9.0
	Natrona	69.0	6.6
	Niobrara	100.0	16.3
	Park	18.9	13.7

State	County	Percent domestic use water from ground water[a,b]	Percent domestic use water self supplied[a,c]
Wyoming, cont.	Sublette	54.6	22.1
	Sweetwater	3.5	0.4
	Uinta	19.5	11.5
	Washakie	100.0	16.0

[a] Data accessed from the USGS website (http://water.usgs.gov/watuse/data/2010/) on November 11, 2014. Domestic water use is water used for indoor household purposes such as drinking, food preparation, bathing, washing clothes and dishes, flushing toilets, and outdoor purposes such as watering lawns and gardens (Maupin et al., 2014).

[b] Percent domestic water use from ground water estimated with the following equation: (Domestic public supply volume from ground water + Domestic self-supplied volume from ground water)/ Domestic total water use volume * 100. Domestic public supply volume from ground water was estimated by multiplying the volume of domestic water from public supply by the ratio of public supply volume from ground water to total public supply volume.

[c] Percent domestic water use self-supplied estimated by dividing the volume of domestic water self-supplied by total domestic water use volume.

Table B-7. Projected hydraulic fracturing water use by Texas counties between 2015 and 2060, expressed as a percentage of 2010 total county water use.

Hydraulic fracturing water use data from Nicot et al. (2012). Total water use data from 2010 from the USGS Water Census (Maupin et al., 2014). All 254 Texas counties are listed by descending order of percentages in 2030.

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
McMullen	126.2	137.0	152.1	165.1	176.7	164.0	145.3	126.6	108.0	89.3
Irion	36.1	59.2	70.5	63.7	53.4	43.1	32.8	22.4	12.1	5.4
La Salle	58.4	58.3	59.7	60.8	61.9	54.6	45.3	36.0	26.7	17.4
San Augustine	60.2	56.2	52.2	48.2	44.2	40.2	36.2	32.1	28.1	24.1
Sterling	12.0	32.0	39.9	40.5	41.0	34.7	28.3	21.9	15.6	10.7
Dimmit	38.2	38.1	38.9	39.0	38.7	33.9	27.9	22.0	16.0	10.1
Sabine	9.6	19.2	28.7	38.3	35.1	31.9	28.7	25.6	22.3	19.2
Leon	9.9	19.3	27.0	34.6	32.9	29.0	25.1	21.2	17.3	13.5
Karnes	48.1	43.0	37.9	32.6	27.2	21.8	16.4	11.0	5.6	0.2
Loving	13.1	17.4	23.4	29.4	28.8	26.2	23.6	20.9	18.3	15.7
Shackelford	0.0	7.9	15.7	23.6	21.2	18.9	16.5	14.1	11.8	9.4
Madison	5.5	11.8	15.7	19.7	17.4	15.2	13.0	10.9	8.7	6.5
Schleicher	10.5	15.8	19.1	19.7	17.1	14.5	11.9	9.3	6.7	4.7
Sutton	0.0	11.0	15.1	19.1	23.2	20.6	18.1	15.5	12.9	10.3
Shelby	11.0	20.4	19.4	18.4	17.4	15.7	14.1	12.5	10.9	9.3
DeWitt	26.9	24.1	21.4	18.4	15.4	12.3	9.3	6.3	3.2	0.2
Hemphill	25.7	23.1	20.5	17.8	15.2	12.6	10.0	7.3	4.7	2.1

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Terrell	0.0	9.7	13.2	16.8	20.4	18.2	15.9	13.6	11.3	9.0
Coryell	7.0	24.4	22.8	16.5	10.1	3.8	0.0	0.0	0.0	0.0
Montague	28.6	24.5	20.4	16.3	12.2	8.2	4.1	0.0	0.0	0.0
Crockett	7.6	12.5	14.8	13.4	11.2	9.1	6.9	4.7	2.5	1.1
Upton	12.1	15.2	14.1	12.9	11.7	9.8	7.9	5.9	4.0	2.7
Borden	3.1	8.6	12.0	12.1	12.2	10.3	8.4	6.4	4.5	3.1
Live Oak	13.3	12.4	11.5	11.8	12.2	12.7	13.2	11.7	9.8	7.8
Reagan	11.2	14.0	12.7	11.3	9.9	8.1	6.4	4.6	2.8	1.6
Clay	3.2	5.9	8.6	11.3	10.3	9.4	8.4	7.5	6.6	5.6
Wheeler	17.6	15.3	13.1	10.8	8.6	6.3	4.1	1.8	0.0	0.0
Lavaca	7.9	13.2	12.0	10.7	9.4	8.1	6.7	5.4	4.0	2.7
Washington	0.0	6.7	11.8	10.7	9.6	8.6	7.5	6.4	5.3	4.3
Nacogdoches	7.9	11.4	10.7	10.0	9.2	8.3	7.5	6.6	5.7	4.9
Hill	17.1	14.7	12.2	9.8	7.3	4.9	2.4	0.0	0.0	0.0
Jack	3.5	5.3	7.1	8.8	7.9	7.1	6.2	5.3	4.4	3.5
Panola	7.2	10.2	9.2	8.5	7.7	7.0	6.3	5.5	4.8	4.0
Jim Hogg	4.8	6.4	8.0	8.0	6.9	6.0	4.9	3.9	2.9	1.8
Howard	4.4	7.1	8.5	8.0	6.8	5.6	4.4	3.2	2.1	1.3
Parker	3.7	5.0	6.3	7.6	6.8	6.1	5.3	4.5	3.8	3.0
Hamilton	8.8	10.7	8.9	7.1	5.3	3.5	1.8	0.0	0.0	0.0
Johnson	14.2	11.9	9.5	7.1	4.7	2.4	0.0	0.0	0.0	0.0
Midland	6.7	8.3	7.7	7.1	6.2	5.2	4.1	3.0	2.0	1.2

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Kenedy	4.1	5.4	6.8	6.8	5.9	5.1	4.1	3.3	2.4	1.6
Fayette	3.9	8.4	7.6	6.6	5.5	4.4	3.4	2.3	1.2	0.2
Lee	2.1	4.1	5.3	6.5	5.8	5.1	4.3	3.6	2.9	2.1
Winkler	2.9	3.8	5.1	6.3	6.0	5.4	4.7	4.1	3.4	2.8
Wilson	6.7	7.7	7.0	6.2	5.4	4.6	3.9	3.1	2.3	1.5
Martin	5.7	7.1	6.5	6.0	5.3	4.4	3.5	2.6	1.8	1.2
Burleson	1.0	2.9	4.3	5.7	5.1	4.5	3.9	3.3	2.6	2.0
Atascosa	6.3	5.7	5.6	5.6	5.6	5.6	5.0	4.2	3.4	2.7
Bosque	1.8	3.0	4.3	5.5	5.1	4.6	4.2	3.7	3.2	2.8
Webb	7.5	7.1	6.3	5.4	4.6	3.8	3.1	2.3	1.4	0.5
Gonzales	8.0	7.1	6.2	5.3	4.4	3.6	2.7	1.8	0.9	0.0
Marion	1.1	2.4	3.8	5.1	5.2	4.7	4.2	3.7	3.2	2.7
Harrison	4.3	6.1	5.5	5.1	4.6	4.2	3.7	3.3	2.9	2.4
Eastland	0.0	3.9	5.9	5.0	4.2	3.3	2.5	1.7	0.8	0.0
Archer	1.0	2.4	3.6	4.9	4.5	4.1	3.7	3.3	2.9	2.5
Zavala	4.7	5.5	5.2	4.9	4.6	4.3	4.0	3.4	2.7	2.0
Roberts	6.9	6.0	5.1	4.2	3.4	2.5	1.6	0.7	0.0	0.0
Maverick	2.5	3.0	3.6	4.2	4.8	4.5	4.0	3.6	3.1	2.6
Cooke	11.9	9.3	6.7	4.1	1.5	0.0	0.0	0.0	0.0	0.0
Ward	2.7	3.2	4.2	4.1	4.0	3.6	3.2	2.7	2.3	1.9
Austin	0.0	1.2	2.5	3.7	3.4	3.0	2.6	2.2	1.9	1.5
Reeves	1.4	1.8	2.7	3.7	3.9	3.6	3.3	3.0	2.6	2.3

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Glasscock	3.1	4.1	3.9	3.6	3.1	2.6	2.1	1.5	1.0	0.7
Tyler	1.9	2.6	3.2	3.2	2.8	2.4	2.0	1.6	1.1	0.7
Hood	1.4	2.0	2.6	3.2	2.9	2.6	2.2	1.9	1.6	1.3
Garza	1.5	2.0	2.5	2.9	2.7	2.4	2.1	1.8	1.5	1.2
Andrews	2.3	3.0	2.9	2.7	2.6	2.3	2.0	1.7	1.4	1.1
Crane	1.3	1.7	2.1	2.6	3.1	2.8	2.5	2.2	1.9	1.7
Erath	0.9	1.4	1.9	2.4	2.2	2.0	1.8	1.6	1.4	1.2
Wise	3.6	3.2	2.8	2.4	2.0	1.6	1.2	0.8	0.4	0.0
Upshur	0.2	0.9	1.7	2.4	2.9	2.6	2.3	2.1	1.8	1.5
Mitchell	1.2	1.6	2.0	2.4	2.1	1.9	1.7	1.4	1.2	0.9
Ector	1.5	2.0	2.1	2.3	2.2	1.9	1.7	1.4	1.2	1.0
Culberson	0.3	0.4	1.3	2.2	2.9	2.6	2.4	2.1	1.9	1.6
Lipscomb	1.7	3.0	2.6	2.1	1.7	1.3	0.8	0.4	0.0	0.0
Angelina	0.4	0.9	1.5	2.1	2.2	2.0	1.8	1.6	1.4	1.2
Houston	2.1	2.7	2.4	2.1	1.8	1.5	1.2	0.9	0.6	0.3
Frio	1.8	1.8	1.9	1.9	1.8	1.8	1.7	1.5	1.2	0.9
Newton	1.8	2.3	2.1	1.8	1.6	1.3	1.0	0.8	0.5	0.3
Kleberg	1.0	1.4	1.7	1.7	1.5	1.3	1.1	0.8	0.6	0.4
Brooks	1.0	1.3	1.7	1.7	1.5	1.2	1.0	0.8	0.6	0.4
Brazos	0.4	0.9	1.2	1.5	1.4	1.2	1.0	0.8	0.7	0.5
Comanche	0.4	0.7	1.0	1.4	1.2	1.1	1.0	0.8	0.7	0.5
Ochiltree	0.6	1.1	1.5	1.2	1.0	0.7	0.5	0.2	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Palo Pinto	0.3	0.6	0.9	1.2	1.1	1.0	0.8	0.7	0.6	0.5
Limestone	0.9	1.0	1.1	1.2	1.1	1.0	0.8	0.7	0.6	0.4
Duval	0.7	0.9	1.1	1.1	1.0	0.8	0.7	0.5	0.4	0.3
Stephens	0.1	0.4	0.8	1.1	1.0	0.9	0.8	0.6	0.5	0.4
Dawson	0.5	0.8	1.0	1.1	1.1	1.0	0.8	0.6	0.5	0.3
Scurry	0.0	0.6	0.8	1.0	1.2	1.1	0.9	0.8	0.7	0.5
Bee	0.8	1.1	1.1	1.0	0.9	0.7	0.6	0.4	0.3	0.1
Val Verde	0.0	0.5	0.8	0.9	1.1	1.0	0.9	0.8	0.6	0.5
Colorado	<0.1	0.3	0.6	0.9	0.8	0.7	0.6	0.5	0.4	0.4
Tarrant	2.1	1.7	1.3	0.9	0.4	0.0	0.0	0.0	0.0	0.0
Zapata	0.5	0.7	0.8	0.8	0.7	0.6	0.5	0.4	0.3	0.2
Ellis	0.3	0.5	0.6	0.8	0.7	0.6	0.6	0.5	0.4	0.3
Jim Wells	0.4	0.6	0.7	0.7	0.6	0.5	0.4	0.4	0.3	0.2
Lynn	0.0	0.4	0.6	0.7	0.8	0.8	0.7	0.6	0.5	0.4
Henderson	0.1	0.3	0.5	0.7	0.8	0.7	0.6	0.5	0.4	0.4
Hansford	0.0	0.4	0.8	0.7	0.5	0.4	0.3	0.2	0.1	0
Gaines	0.2	0.3	0.5	0.5	0.5	0.4	0.4	0.3	0.2	0.2
Gregg	0.1	0.2	0.3	0.4	0.4	0.4	0.4	0.3	0.3	0.2
Refugio	0.2	0.3	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Caldwell	0.4	0.5	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Pecos	0.1	0.1	0.2	0.4	0.5	0.4	0.4	0.3	0.3	0.2
Anderson	0.1	0.2	0.3	0.4	0.4	0.4	0.4	0.3	0.3	0.2

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Young	0.0	0.1	0.2	0.4	0.3	0.3	0.3	0.2	0.2	0.1
San Patricio	0.2	0.3	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Smith	0.1	0.1	0.2	0.3	0.4	0.3	0.3	0.3	0.2	0.2
Cherokee	0.1	0.2	0.2	0.3	0.4	0.3	0.3	0.2	0.2	0.2
McLennan	0.1	0.1	0.2	0.3	0.3	0.2	0.2	0.2	0.2	0.1
Terry	0.0	0.2	0.2	0.3	0.3	0.3	0.3	0.2	0.2	0.2
Starr	0.2	0.2	0.3	0.3	0.2	0.2	0.2	0.1	0.1	0.1
Cochran	0.1	0.2	0.2	0.2	0.3	0.2	0.2	0.2	0.2	0.1
Jasper	0.2	0.3	0.2	0.2	0.2	0.1	0.1	0.1	0.1	<0.1
Dallas	0.2	0.3	0.2	0.2	0.1	0.1	<0.1	0.0	0.0	0.0
Robertson	0.1	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.1	0.1
Grimes	<0.1	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.1
Yoakum	0.1	0.1	0.2	0.2	0.1	0.1	0.1	0.1	0.1	0.1
Freestone	0.1	0.1	0.1	0.2	0.2	0.1	0.1	0.1	0.1	0.1
Cass	<0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.1	0.1	0.1
Hutchinson	0.0	0.1	0.2	0.1	0.1	0.1	0.1	<0.1	<0.1	0.0
Rusk	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	<0.1
Willacy	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1
Victoria	<0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Sherman	0.0	0.0	<0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Calhoun	<0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Lubbock	0.0	0.0	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Jackson	<0.1	<0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Matagorda	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Polk	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Wharton	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Nueces	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Hidalgo	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Cameron	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Somervell	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Goliad	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Brazoria	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Fort Bend	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Aransas	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Armstrong	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bailey	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bandera	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bastrop	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Baylor	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bell	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bexar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Blanco	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bowie	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Brewster	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Briscoe	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Brown	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Burnet	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Callahan	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Camp	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Carson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Castro	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chambers	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Childress	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Coke	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Coleman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Collin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Collingsworth	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Comal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Concho	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cottle	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Crosby	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dallam	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Deaf Smith	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Delta	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Denton	1.7	1.1	0.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dickens	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Donley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Edwards	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
El Paso	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Falls	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fannin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fisher	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Floyd	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Foard	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Franklin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Galveston	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Gillespie	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Gray	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Grayson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Guadalupe	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hale	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hardeman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hardin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Harris	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hartley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Haskell	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hays	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Hockley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hopkins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hudspeth	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hunt	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jeff Davis	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jefferson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jones	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kaufman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kendall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kent	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kerr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kimble	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
King	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kinney	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Knox	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lamar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lamb	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lampasas	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Liberty	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Llano	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
McCulloch	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mason	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Medina	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Menard	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Milam	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mills	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Montgomery	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Moore	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Morris	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Motley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Navarro	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Nolan	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Oldham	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Orange	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Parmer	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Potter	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Presidio	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Rains	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Randall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Real	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Red River	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Rockwall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Runnels	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
San Jacinto	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use[a,b]									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
San Saba	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Stonewall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Swisher	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Taylor	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Throckmorton	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Titus	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Tom Green	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Travis	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Trinity	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Uvalde	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Van Zandt	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Walker	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Waller	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wichita	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wilbarger	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Williamson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wood	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

[a] Total water use data accessed from the USGS website (http://water.usgs.gov/watuse/data/2010/) on April 21, 2015. Data from Nicot et al. (2012) transcribed.

[b] Percentages calculated by dividing projected hydraulic fracturing water use volumes from Nicot et al. (2012) by 2010 total water use from the USGS and multiplying by 100. Percentages less than 0.1 were not rounded and simply noted as "<0.1", but where the percentage was actually zero because there was no projected hydraulic fracturing water use we noted that as "0.0".

B.2. References for Appendix B

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Appendix C

Chemical Mixing Supplemental Tables and Information

Appendix C. Chemical Mixing Supplemental Tables and Information

C.1. Supplemental Tables and Information

Table C-1. Chemicals reported to FracFocus in 10% or more of disclosures for gas-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.

Chemicals ranked by frequency of occurrence (U.S. EPA, 2015c).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Hydrochloric acid	7647-01-0	12,351	72.8%	15%
Methanol	67-56-1	12,269	72.3%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	11,897	70.1%	30%
Isopropanol	67-63-0	8,008	47.2%	30%
Water	7732-18-5	7,998	47.1%	63%
Ethanol	64-17-5	6,325	37.3%	5%
Propargyl alcohol	107-19-7	5,811	34.2%	10%
Glutaraldehyde	111-30-8	5,635	33.2%	30%
Ethylene glycol	107-21-1	5,493	32.4%	35%
Citric acid	77-92-9	4,832	28.5%	60%
Sodium hydroxide	1310-73-2	4,656	27.4%	5%
Peroxydisulfuric acid, diammonium salt	7727-54-0	4,618	27.2%	100%
Quartz	14808-60-7	3,758	22.1%	10%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	3,668	21.6%	100%
Sodium chloride	7647-14-5	3,608	21.3%	30%
Guar gum	9000-30-0	3,586	21.1%	60%
Acetic acid	64-19-7	3,563	21.0%	50%
2-Butoxyethanol	111-76-2	3,325	19.6%	10%
Naphthalene	91-20-3	3,294	19.4%	5%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,287	19.4%	30%
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	3,259	19.2%	7%
Potassium hydroxide	1310-58-3	2,843	16.8%	15%
Ammonium chloride	12125-02-9	2,483	14.6%	10%
Choline chloride	67-48-1	2,477	14.6%	75%

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	2,455	14.5%	5%
Sodium chlorite	7758-19-2	2,372	14.0%	10%
1,2,4-Trimethylbenzene	95-63-6	2,229	13.1%	1%
Carbonic acid, dipotassium salt	584-08-7	2,154	12.7%	60%
Methenamine	100-97-0	2,134	12.6%	1%
Formic acid	64-18-6	2,118	12.5%	60%
Didecyl dimethyl ammonium chloride	7173-51-5	2,063	12.2%	10%
N,N-Dimethylformamide	68-12-2	1,892	11.2%	13%
Phenolic resin	9003-35-4	1,852	10.9%	5%
Thiourea polymer	68527-49-1	1,702	10.0%	30%
Polyethylene glycol	25322-68-3	1,696	10.0%	60%

Note: Analysis considered 17,035 disclosures and 291,363 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (1,587) or other, query-specific criteria were excluded from analysis.

Table C-2. Chemicals reported to FracFocus in 10% or more of disclosures for oil-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.

Chemicals ranked by frequency of occurrence (U.S. EPA, 2015c).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Methanol	67-56-1	12,484	71.8%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	10,566	60.8%	40%
Peroxydisulfuric acid, diammonium salt	7727-54-0	10,350	59.6%	100%
Ethylene glycol	107-21-1	10,307	59.3%	30%
Hydrochloric acid	7647-01-0	10,029	57.7%	15%
Guar gum	9000-30-0	9,110	52.4%	50%
Sodium hydroxide	1310-73-2	8,609	49.5%	10%
Quartz	14808-60-7	8,577	49.4%	2%
Water	7732-18-5	8,538	49.1%	67%
Isopropanol	67-63-0	8,031	46.2%	15%
Potassium hydroxide	1310-58-3	7,206	41.5%	15%
Glutaraldehyde	111-30-8	5,927	34.1%	15%
Propargyl alcohol	107-19-7	5,599	32.2%	5%
Acetic acid	64-19-7	4,623	26.6%	30%
2-Butoxyethanol	111-76-2	4,022	23.1%	10%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,821	22.0%	5%
Sodium chloride	7647-14-5	3,692	21.2%	25%
Ethanol	64-17-5	3,536	20.3%	45%
Citric acid	77-92-9	3,310	19.0%	60%
Phenolic resin	9003-35-4	3,109	17.9%	5%
Naphthalene	91-20-3	3,060	17.6%	5%
Nonyl phenol ethoxylate	9016-45-9	2,829	16.3%	20%
Diatomaceous earth, calcined	91053-39-3	2,655	15.3%	100%
Methenamine	100-97-0	2,559	14.7%	1%
Tetramethylammonium chloride	75-57-0	2,428	14.0%	1%
Carbonic acid, dipotassium salt	584-08-7	2,402	13.8%	60%
Ethoxylated propoxylated C12-14 alcohols	68439-51-0	2,342	13.5%	2%
Choline chloride	67-48-1	2,264	13.0%	75%
Boron sodium oxide	1330-43-4	2,228	12.8%	30%
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	2,130	12.3%	50%
1,2,4-Trimethylbenzene	95-63-6	2,118	12.2%	1%

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Boric acid	10043-35-3	2,070	11.9%	25%
Polyethylene glycol	25322-68-3	2,025	11.7%	5%
2-Mercaptoethanol	60-24-2	2,012	11.6%	100%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,988	11.4%	98%
Formic acid	64-18-6	1,948	11.2%	60%
Sodium persulfate	7775-27-1	1,914	11.0%	100%
Phosphonic acid	13598-36-2	1,865	10.7%	1%
Sodium tetraborate decahydrate	1303-96-4	1,862	10.7%	30%
Potassium metaborate	13709-94-9	1,682	9.7%	60%
Ethylenediaminetetraacetic acid tetrasodium salt hydrate	64-02-8	1,676	9.6%	0%
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	1,668	9.6%	5%

Note: Analysis considered 17,640 disclosures and 385,013 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (2,268) or other, query-specific criteria were excluded from analysis.

Table C-3a. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, Alabama to Montana (U.S. EPA, 2015c).

Source: (U.S. EPA, 2015c). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Methanol	67-56-1	55 (100%)		1333 (99.7%)	228 (39.0%)	2883 (63.3%)	77 (79.4%)	596 (59.2%)	13 (92.9%)	3 (75%)	121 (62.7%)
Distillates, petroleum, hydrotreated light	64742-47-8		9 (45%)	743 (55.6%)	322 (55.0%)	3358 (73.7%)	87 (89.7%)	844 (83.9%)	14 (100%)	4 (100%)	115 (59.6%)
Ethylene glycol	107-21-1	55 (100%)	20 (100%)	291 (21.8%)	350 (59.8%)		61 (62.9%)	341 (33.9%)	10 (71.4%)	3 (75%)	95 (49.2%)
Isopropanol	67-63-0	55 (100%)	13 (65%)	586 (43.9%)		2586 (56.8%)	24 (24.7%)	515 (51.2%)	11 (78.6%)		123 (63.7%)
Quartz	14808-60-7		20 (100%)		519 (88.7%)	1048 (23.0%)	22 (22.7%)	377 (37.5%)		2 (50%)	124 (64.2%)
Sodium hydroxide	1310-73-2		20 (100%)	285 (21.3%)	403 (68.9%)	996 (21.9%)	27 (27.8%)	535 (53.2%)		2 (50%)	105 (54.4%)
Ethanol	64-17-5			603 (45.1%)		2258 (49.6%)	78 (80.4%)	420 (41.7%)		4 (100%)	
Guar gum	9000-30-0		10 (50%)		545 (93.2%)			494 (49.1%)		2 (50%)	83 (43.0%)
Hydrochloric acid	7647-01-0	55 (100%)		1330 (99.5%)		2408 (52.9%)	82 (84.5%)	569 (56.6%)			45 (23.3%)
Peroxydisulfuric acid, diammonium salt	7727-54-0		10 (50%)		484 (82.7%)		21 (21.6%)	273 (27.2%)	8 (57.1%)		119 (61.7%)

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Propargyl alcohol	107-19-7			813 (60.8%)			69 (71.1%)	299 (29.7%)	5 (35.7%)		
Glutaraldehyde	111-30-8			737 (55.1%)			73 (75.3%)	364 (36.3%)		2 (50%)	
Naphthalene	91-20-3	55 (100%)				1363 (29.9%)	41 (42.3%)	293 (29.2%)	12 (85.7%)		95 (49.2%)
2-Butoxyethanol	111-76-2	55 (100%)	20 (100%)						11 (78.6%)		
Citric acid	77-92-9						45 (46.4%)				
Saline	7647-14-5					1574 (34.5%)		408 (40.6%)		2 (50%)	
Solvent naphtha, petroleum, heavy arom.	64742-94-5					1507 (33.1%)	42 (43.3%)				135 (70.0%)
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1			375 (28.0%)			52 (53.6%)			2 (50%)	
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	55 (100%)				2215 (48.6%)			10 (71.4%)		70 (36.3%)
Potassium hydroxide	1310-58-3							340 (33.8%)		4 (100%)	115 (59.6%)
Choline chloride	67-48-1					1235 (27.1%)					
Polyethylene glycol	25322-68-3	55 (100%)							7 (50%)		69 (35.8%)
1,2,4-Trimethylbenzene	95-63-6					1211 (26.63%)	39 (40.2%)				

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Ammonium chloride	12125-02-9			277 (20.7%)		1280 (28.0%)					
Diatomaceous earth, calcined	91053-39-3		20 (100%)		417 (71.3%)						
Didecyl dimethyl ammonium chloride	7173-51-5			317 (23.7%)						2 (50%)	
Sodium chlorite	7758-19-2							352 (35.0%)		4 (100%)	
Sodium erythorbate	6381-77-7			435 (32.5%)			29 (29.9%)				
N,N-Dimethylformamide	68-12-2										
Nonyl phenol ethoxylate	9016-45-9										
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0				1150 (25.2%)	39 (40.2%)					
Sodium persulfate	7775-27-1									4 (100%)	
Tetramethylammonium chloride	75-57-0										85 (44.0%)
1,2-Propylene glycol	57-55-6								10 (71.4%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4		20 (100%)		389 (66.5%)						
Acetic acid	64-19-7					959 (21.0%)		284 (28.2%)			
Ammonium acetate	631-61-8									2 (50%)	

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Boric acid	10043-35-3		3 (15%)								
Carbonic acid, dipotassium salt	584-08-7					1159 (25.4%)					
Cristobalite	14464-46-1		20 (100%)		389 (66.5%)						
Formic acid	64-18-6	55 (100%)						293 (29.1%)			
Hemicellulase enzyme	9012-54-8										
Hemicellulase enzyme concentrate	9025-56-3				395 (67.5%)						
Iron(II) sulfate heptahydrate	7782-63-0								7 (50%)		
Magnesium chloride	7786-30-3		20 (100%)		389 (66.5%)						
Magnesium nitrate	10377-60-3		20 (100%)		389 (66.5%)						
Phenolic resin	9003-35-4										
Sodium hypochlorite	7681-52-9					1046 (23.0%)					
Sodium tetraborate decahydrate	1303-96-4		14 (70%)								
Solvent naphtha, petroleum, heavy aliph.	64742-96-7								7 (50%)	2 (50%)	
1-Butoxy-2-propanol	5131-66-8				315 (53.8%)						

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
1-Propanol	71-23-8					1232 (27.0%)					
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-,tetrachloride	138879-94-4			343 (58.6%)							
2-bromo-3-nitrilopropionamide	1113-55-9										
2-Ethylhexanol	104-76-7										83 (43.0052%)
2-Methyl-3(2H)-isothiazolone	2682-20-4		20 (100%)		389 (66.5%)						
2-Propenoic acid, polymer with 2-propenamide	9003-06-9										
Alkenes, C>10 .alpha.-	64743-02-8			241 (18.0%)							
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										50 (25.9%)
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										48 (24.9%)
Benzyldimethyldodecylammonium chloride	139-07-1			268 (20.0%)							

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Benzylhexadecyldimethylammonium chloride	122-18-9			268 (20.0%)							
Boron sodium oxide	1330-43-4				361 (61.7%)						
C10-C16 ethoxylated alcohol	68002-97-1		3 (15%)								
Calcium chloride	10043-52-4		20 (100%)								
Carbon dioxide	124-38-9								7 (50%)		
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	55 (100%)									
Diethylene glycol	111-46-6										
Diethylene glycol monobutyl ether	112-34-5								7 (50%)		
Diethylenetriamine	111-40-0										55 (28.5%)
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8				314 (53.7%)						
Distillates, petroleum, hydrotreated middle	64742-46-7		3 (15%)								
Ethoxylated C12-16 alcohols	68551-12-2										
Ethoxylated C14-15 alcohols	68951-67-7			241 (18.0%)							
Formic acid, potassium salt	590-29-4										

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Glycerin, natural	56-81-5								7 (50%)		
Isotridecanol, ethoxylated	9043-30-5				312 (53.3%)						
Methenamine	100-97-0							298 (29.6%)			
Naphtha, petroleum, hydrotreated heavy	64742-48-9										
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8								9 (64.3%)		
Potassium chloride	7447-40-7								7 (50%)		
Sodium bromate	7789-38-0								7 (50%)		
Sodium perborate tetrahydrate	10486-00-7										
Sulfamic acid	5329-14-6									2 (50%)	
Terpenes and Terpenoids, sweet orange-oil	68647-72-3									2 (50%)	
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2			268 (20.0%)							
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8										

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Thiourea polymer	68527-49-1			384 (28.7%)							
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8										
Trisodium phosphate	7601-54-9						19 (19.6%)				

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

Table C-3b. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, New Mexico to Wyoming (U.S. EPA, 2015c).

Source: (U.S. EPA, 2015c). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Methanol	67-56-1	1012 (90.8%)	1059 (53.3%)	76 (52.1%)	1270 (70.3%)	1633 (68.6%)	12664 (78.5%)	984 (78.5%)	48 (60.8%)	153 (64.0%)	460 (38.4%)
Distillates, petroleum, hydrotreated light	64742-47-8	699 (62.7%)	943 (47.5%)	122 (83.6%)	1270 (70.3%)	1434 (60.2%)	10677 (66.1%)	934 (74.5%)		196 (82.0%)	612 (51.1%)
Ethylene glycol	107-21-1	503 (45.1%)	724 (36.4%)	83 (56.8%)	843 (46.7%)	807 (33.9%)	9591 (59.4%)	1065 (85.0%)	22 (27.8%)	141 (59.0%)	
Isopropanol	67-63-0	695 (62.3%)	739 (37.2%)	71 (48.6%)	764 (42.28%)	735 (30.9%)	7731 (47.9%)	661 (52.8%)	43 (54.4%)	74 (31.0%)	516 (43.1%)

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quartz	14808-60-7	762 (68.3%)	920 (46.3%)	66 (45.2%)	491 (27.2%)		6869 (42.6%)	503 (40.1%)		53 (22.2%)	356 (29.7%)
Sodium hydroxide	1310-73-2	329 (29.5%)	1028 (51.7%)		490 (27.1%)	406 (17.0%)	7371 (45.7%)	466 (37.2%)			688 (57.4%)
Ethanol	64-17-5	529 (47.4%)	545 (27.4%)	87 (59.6%)	838 (46.4%)	388 (16.3%)	3439 (21.3%)		50 (63.3%)	130 (54.3%)	298 (24.9%)
Guar gum	9000-30-0	702 (63.0%)	1094 (55.1%)	74 (50.7%)	457 (25.3%)	538 (22.6%)	6863 (42.5%)	538 (42.9%)		55 (23.0%)	823 (68.7%)
Hydrochloric acid	7647-01-0	880 (78.9%)		145 (99.3%)	1372 (75.9%)	2279 (95.7%)	11424 (70.8%)	1064 (84.9%)	68 (86.1%)	229 (95.8%)	
Peroxydisulfuric acid, diammonium salt	7727-54-0	836 (75.0%)	1089 (54.8%)	93 (63.7%)	713 (39.5%)		8666 (53.7%)	483 (38.5%)		128 (53.6%)	771 (64.4%)
Propargyl alcohol	107-19-7	760 (68.2%)		72 (49.3%)	732 (40.5%)	1371 (57.6%)	6269 (38.8%)	456 (36.4%)	22 (27.8%)	138 (57.7%)	
Glutaraldehyde	111-30-8	632 (56.7%)		105 (71.9%)	989 (54.7%)	819 (34.4%)	6470 (40.1%)			169 (70.7%)	260 (21.7%)
Naphthalene	91-20-3		864 (43.5%)		448 (24.8%)			478 (38.1%)	7 (8.9%)		
2-Butoxyethanol	111-76-2	412 (37.0%)				498 (20.9%)	3898 (24.1%)	663 (52.9%)	70 (88.6%)	62 (25.9%)	
Citric acid	77-92-9	447 (40.1%)		96 (65.8%)	644 (35.6%)	701 (29.4%)	3820 (23.7%)	992 (79.2%)	63 (79.8%)	98 (41.0%)	
Saline	7647-14-5		491 (24.7%)				3462 (21.4%)		7 (8.9%)	53 (22.2%)	274 (22.9%)
Solvent naphtha, petroleum, heavy arom.	64742-94-5		981 (49.4%)		557 (30.8%)		2751 (17.0%)		7 (8.9%)		415 (34.6%)

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1			54 (37.0%)	597 (33.0%)	373 (15.7%)				53 (22.2%)	
2,2-Dibromo-3-nitrilopropionamide	10222-01-2					804 (33.8%)			22 (27.8%)		
Potassium hydroxide	1310-58-3		1176 (59.2%)	106 (72.6%)			6369 (39.5%)				
Choline chloride	67-48-1	384 (34.4%)		55 (37.7%)				649 (51.8%)	45 (57.0%)		
Polyethylene glycol	25322-68-3		567 (28.5%)			688 (28.9%)					
1,2,4-Trimethylbenzene	95-63-6		496 (25.0%)						7 (8.9%)		
Ammonium chloride	12125-02-9					732 (30.7%)				50 (20.9%)	
Diatomaceous earth, calcined	91053-39-3	419 (37.6%)						435 (34.7%)			
Didecyl dimethyl ammonium chloride	7173-51-5			46 (31.6%)						49 (20.5%)	
Sodium chlorite	7758-19-2		482 (24.3%)								271 (22.6%)
Sodium erythorbate	6381-77-7								10 (12.7%)	76 (31.8%)	
N,N-Dimethylformamide	68-12-2			68 (46.6%)	355 (19.6%)			410 (32.7%)			
Nonyl phenol ethoxylate	9016-45-9	333 (29.9%)						447 (35.7%)	25 (31.6%)		

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0								7 (8.9%)		
Sodium persulfate	7775-27-1					373 (15.7%)					308 (25.7%)
Tetramethylammonium chloride	75-57-0		579 (29.1%)								315 (26.3%)
1,2-Propylene glycol	57-55-6								22 (27.8%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4										
Acetic acid	64-19-7										
Ammonium acetate	631-61-8										323 (27.0%)
Boric acid	10043-35-3			82 (56.2%)							
Carbonic acid, dipotassium salt	584-08-7		482 (24.2%)								
Cristobalite	14464-46-1										
Formic acid	64-18-6										
Hemicellulase enzyme	9012-54-8					367 (15.4%)			11 (13.9%)		
Hemicellulase enzyme concentrate	9025-56-3	331 (29.7%)									
Iron(II) sulfate heptahydrate	7782-63-0								22 (27.8%)		
Magnesium chloride	7786-30-3										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Magnesium nitrate	10377-60-3										
Phenolic resin	9003-35-4	419 (37.6%)					2903 (18.0%)				
Sodium hypochlorite	7681-52-9										282 (23.5%)
Sodium tetraborate decahydrate	1303-96-4										265 (22.1%)
Solvent naphtha, petroleum, heavy aliph.	64742-96-7										
1-Butoxy-2-propanol	5131-66-8										
1-Propanol	71-23-8										
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxy ethyl) methylammonio] ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4										
2-Bromo-3-nitrilopropionamide	1113-55-9								11 (13.9%)		
2-Ethylhexanol	104-76-7										
2-Methyl-3(2H)-isothiazolone	2682-20-4										
2-Propenoic acid, polymer with 2-propenamide	9003-06-9							486 (38.8%)			
Alkenes, C>10 .alpha.-	64743-02-8										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										
Benzyldimethyldodecylammonium chloride	139-07-1										
Benzylhexadecyldimethylammonium chloride	122-18-9										
Boron sodium oxide	1330-43-4										
C10-C16 ethoxylated alcohol	68002-97-1										
Calcium chloride	10043-52-4										
Carbon dioxide	124-38-9										
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2										
Diethylene glycol	111-46-6			45 (30.8%)							
Diethylene glycol monobutyl ether	112-34-5										
Diethylenetriamine	111-40-0										
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Distillates, petroleum, hydrotreated middle	64742-46-7										
Ethoxylated C12-16 alcohols	68551-12-2									57 (23.8%)	
Ethoxylated C14-15 alcohols	68951-67-7										
Formic acid, potassium salt	590-29-4										361 (30.1%)
Glycerin, natural	56-81-5										
Isotridecanol, ethoxylated	9043-30-5										
Methenamine	100-97-0										
Naphtha, petroleum, hydrotreated heavy	64742-48-9										384 (32.1%)
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8										
Potassium chloride	7447-40-7										
Sodium bromate	7789-38-0										
Sodium perborate tetrahydrate	10486-00-7				351 (19.4%)						
Sulfamic acid	5329-14-6										
Terpenes and terpenoids, sweet orange-oil	68647-72-3										

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2										
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8							945 (75.4%)			
Thiourea polymer	68527-49-1										
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8					350 (14.7%)					
Trisodium phosphate	7601-54-9										

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

Table C-4. Estimated mean, median, 5th percentile, and 95th percentile volumes in gallons for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	2,702	406	0	19,741
1-Butoxy-2-propanol	5131-66-8	167	21	5	654
1-Decanol	112-30-1	28	4	0	33
1-Octanol	111-87-5	5	4	0	10
1-Propanol	71-23-8	128	55	6	367
1,2-Propylene glycol	57-55-6	13,105	72	4	61,071
1,2,4-Trimethylbenzene	95-63-6	38	6	0	43
2-Butoxyethanol	111-76-2	385	26	0	1,811
2-Ethylhexanol	104-76-7	100	11	0	292
2-Mercaptoethanol	60-24-2	1,175	445	0	4,194
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	183	5	0	341
Acetic acid	64-19-7	646	47	0	1,042
Acetic anhydride	108-24-7	239	50	3	722
Acrylamide	79-06-1	95	3	0	57
Adipic acid	124-04-9	153	0	0	109
Aluminum chloride	7446-70-0	2	0	0	0
Ammonia	7664-41-7	44	35	2	138
Ammonium acetate	631-61-8	839	117	0	1,384
Ammonium chloride	12125-02-9	440	48	3	458
Ammonium hydroxide	1336-21-6	7	2	0	14
Benzyl chloride	100-44-7	52	0	0	40
Carbonic acid, dipotassium salt	584-08-7	467	113	0	1,729
Chlorine dioxide	10049-04-4	31	11	0	28
Choline chloride	67-48-1	2,131	290	28	4,364
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	68	3	0	697

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Citric acid	77-92-9	163	20	1	269
Dibromoacetonitrile	3252-43-5	22	13	1	45
Diethylene glycol	111-46-6	168	16	0	102
Diethylenetriamine	111-40-0	92	21	0	207
Dodecane	112-40-3	190	31	0	151
Ethanol	64-17-5	831	121	1	2,645
Ethanolamine	141-43-5	70	30	0	283
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	614	184	4	2,470
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	200	0	0	8
Formic acid	64-18-6	501	38	1	1,229
Fumaric acid	110-17-8	2	0	0	12
Glutaraldehyde	111-30-8	1,313	122	2	1,165
Glycerin, natural	56-81-5	413	109	10	911
Glycolic acid	79-14-1	38	10	4	94
Hydrochloric acid	7647-01-0	28,320	3,110	96	26,877
Isopropanol	67-63-0	2,095	55	0	1,264
Isopropylamine	75-31-0	83	121	0	172
Magnesium chloride	7786-30-3	14	0	0	2
Methanol	67-56-1	1,218	110	2	3,731
Methenamine	100-97-0	3,386	100	0	3,648
Methoxyacetic acid	625-45-6	36	4	2	115
N,N-Dimethylformamide	68-12-2	119	10	0	216
Naphthalene	91-20-3	72	12	0	204
Nitrogen, liquid	7727-37-9	41,841	26,610	3,091	108,200
Ozone	10028-15-6	15,844	15,473	8,785	26,063
Peracetic acid	79-21-0	300	268	50	663
Phosphonic acid	13598-36-2	1,201	0	0	3
Phosphoric acid Divosan X-Tend formulation	7664-38-2	13	4	0	15
Potassium acetate	127-08-2	204	1	0	974

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Propargyl alcohol	107-19-7	183	2	0	51
Saline	7647-14-5	876	85	0	1,544
Saturated sucrose	57-50-1	1	1	0	2
Silica, amorphous	7631-86-9	6,877	8	0	38,371
Sodium carbonate	497-19-8	228	16	0	1,319
Sodium formate	141-53-7	0	0	0	0
Sodium hydroxide	1310-73-2	551	38	0	1,327
Sulfur dioxide	7446-09-5	0	0	0	0
Sulfuric acid	7664-93-9	3	0	0	3
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	156	64	0	557
Tetramethylammonium chloride	75-57-0	970	483	2	3,508
Thioglycolic acid	68-11-1	55	7	2	229
Toluene	108-88-3	18	0	0	11
Tridecane	629-50-5	190	31	0	190
Triethanolamine	102-71-6	846	60	0	2,264
Triethyl phosphate	78-40-0	55	1	0	533
Triethylene glycol	112-27-6	5,198	116	28	945
Triisopropanolamine	122-20-3	46	4	1	330
Trimethyl borate	121-43-7	83	40	4	283
Undecane	1120-21-4	273	29	0	1,641

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-5. Estimated mean, median, 5th percentile, and 95th percentile volumes in liters for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	10,229	1,536	0	74,729
1-Butoxy-2-propanol	5131-66-8	631	80	18	2,475
1-Decanol	112-30-1	107	14	1	123
1-Octanol	111-87-5	21	14	1	39
1-Propanol	71-23-8	483	208	22	1,391
1,2-Propylene glycol	57-55-6	49,607	274	15	231,179
1,2,4-Trimethylbenzene	95-63-6	145	24	0	165
2-Butoxyethanol	111-76-2	1,459	98	0	6,856
2-Ethylhexanol	104-76-7	377	40	1	1,106
2-Mercaptoethanol	60-24-2	4,449	1,685	0	15,878
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	692	18	0	1,292
Acetic acid	64-19-7	2,446	176	0	3,945
Acetic anhydride	108-24-7	906	189	12	2,734
Acrylamide	79-06-1	361	10	0	216
Adipic acid	124-04-9	578	0	0	414
Aluminum chloride	7446-70-0	6	0	0	0
Ammonia	7664-41-7	166	134	7	523
Ammonium acetate	631-61-8	3,177	444	0	5,238
Ammonium chloride	12125-02-9	1,666	182	11	1,733
Ammonium hydroxide	1336-21-6	27	6	1	52
Benzyl chloride	100-44-7	196	1	0	151
Carbonic acid, dipotassium salt	584-08-7	1,769	429	0	6,544
Chlorine dioxide	10049-04-4	117	43	1	106
Choline chloride	67-48-1	8,068	1,096	107	16,521
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	258	12	0	2,638
Citric acid	77-92-9	618	77	5	1,019

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Dibromoacetonitrile	3252-43-5	82	50	4	170
Diethylene glycol	111-46-6	636	61	1	384
Diethylenetriamine	111-40-0	347	80	0	785
Dodecane	112-40-3	719	117	0	572
Ethanol	64-17-5	3,144	458	6	10,011
Ethanolamine	141-43-5	264	112	0	1,070
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	2,324	697	14	9,349
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	756	2	0	31
Formic acid	64-18-6	1,896	144	2	4,653
Fumaric acid	110-17-8	9	0	0	46
Glutaraldehyde	111-30-8	4,972	462	6	4,409
Glycerin, natural	56-81-5	1,565	412	38	3,447
Glycolic acid	79-14-1	146	39	14	356
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741
Isopropanol	67-63-0	7,932	210	1	4,786
Isopropylamine	75-31-0	314	458	0	652
Magnesium chloride	7786-30-3	52	0	0	8
Methanol	67-56-1	4,609	416	6	14,125
Methenamine	100-97-0	12,817	378	0	13,810
Methoxyacetic acid	625-45-6	136	17	8	436
N,N-Dimethylformamide	68-12-2	449	38	2	819
Naphthalene	91-20-3	271	44	0	774
Nitrogen, liquid	7727-37-9	158,384	100,731	11,700	409,583
Ozone	10028-15-6	59,976	58,570	33,254	98,658
Peracetic acid	79-21-0	1,137	1,016	190	2,511
Phosphonic acid	13598-36-2	4,547	2	0	11
Phosphoric acid Divosan X-Tend formulation	7664-38-2	51	15	0	57
Potassium acetate	127-08-2	775	3	0	3,690
Propargyl alcohol	107-19-7	693	9	0	193

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Saline	7647-14-5	3,317	321	0	5,844
Saturated sucrose	57-50-1	5	2	0	6
Silica, amorphous	7631-86-9	26,031	32	0	145,251
Sodium carbonate	497-19-8	862	62	0	4,991
Sodium formate	141-53-7	1	1	0	1
Sodium hydroxide	1310-73-2	2,087	144	1	5,024
Sulfur dioxide	7446-09-5	2	0	0	0
Sulfuric acid	7664-93-9	10	0	0	12
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	591	242	0	2,109
Tetramethylammonium chloride	75-57-0	3,672	1,830	8	13,279
Thioglycolic acid	68-11-1	208	28	6	868
Toluene	108-88-3	69	0	0	41
Tridecane	629-50-5	721	118	0	721
Triethanolamine	102-71-6	3,203	228	0	8,570
Triethyl phosphate	78-40-0	209	6	0	2,019
Triethylene glycol	112-27-6	19,676	439	106	3,579
Triisopropanolamine	122-20-3	174	16	4	1,249
Trimethyl borate	121-43-7	314	152	16	1,072
Undecane	1120-21-4	1,035	111	0	6,212

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-6. Calculated mean, median, 5th percentile, and 95th percentile chemical masses reported to FracFocus in 100 or more disclosures, where density information was available.

Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7. Number of disclosures reported for each chemical is also included.

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	8,593	1,290	0	62,772	578
1-Butoxy-2-propanol	5131-66-8	555	71	16	2,178	773
1-Decanol	112-30-1	89	12	1	102	434
1-Octanol	111-87-5	17	12	1	32	434
1-Propanol	71-23-8	386	167	18	1,113	1,481
1,2-Propylene glycol	57-55-6	51,095	282	15	238,114	1,023
1,2,4-Trimethylbenzene	95-63-6	126	21	0	143	3,976
2-Butoxyethanol	111-76-2	1,313	88	0	6,170	6,778
2-Ethylhexanol	104-76-7	313	34	0	918	1,291
2-Mercaptoethanol	60-24-2	489	185	0	1,747	2,051
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,660	44	0	3,102	4,927
Acetic acid	64-19-7	2,544	183	0	4,103	7,643
Acetic anhydride	108-24-7	969	203	12	2,925	1,377
Acrylamide	79-06-1	408	11	0	244	251
Adipic acid	124-04-9	785	0	0	564	233
Aluminum chloride	7446-70-0	15	0	0	0	122
Ammonia	7664-41-7	111	90	4	351	398
Ammonium acetate	631-61-8	3,718	520	0	6,129	1,504
Ammonium chloride	12125-02-9	2,530	277	16	2,633	3,288
Ammonium hydroxide	1336-21-6	48	11	2	94	1,173
Benzyl chloride	100-44-7	214	1	0	165	1,833
Carbonic acid, dipotassium salt	584-08-7	4,298	1,042	0	15,902	4,093
Chlorine dioxide	10049-04-4	321	117	3	291	331
Choline chloride	67-48-1	9,440	1,282	125	19,329	4,241
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	284	13	0	2,902	1,377

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Citric acid	77-92-9	989	123	8	1,630	7,503
Dibromoacetonitrile	3252-43-5	193	118	11	403	272
Diethylene glycol	111-46-6	712	68	1	430	1,732
Diethylenetriamine	111-40-0	330	76	0	746	784
Dodecane	112-40-3	539	88	0	429	131
Ethanol	64-17-5	2,484	361	4	7,908	9,233
Ethanolamine	141-43-5	267	113	0	1,081	585
Ethyl acetate	141-78-6	0	0	0	0	110
Ethylene glycol	107-21-1	2,557	767	15	10,283	14,767
Ferric chloride	7705-08-0	0	0	0	0	118
Formalin	50-00-0	816	2	0	34	456
Formic acid	64-18-6	2,313	176	2	5,677	3,781
Fumaric acid	110-17-8	15	0	0	75	224
Glutaraldehyde	111-30-8	4,972	462	6	4,409	10,963
Glycerin, natural	56-81-5	1,972	519	47	4,343	1,829
Glycolic acid	79-14-1	217	58	21	530	595
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741	20,996
Isopropanol	67-63-0	6,187	163	1	3,733	15,058
Isopropylamine	75-31-0	213	311	0	444	255
Magnesium chloride	7786-30-3	120	1	0	18	1,113
Methanol	67-56-1	3,641	329	5	11,159	23,225
Methenamine	100-97-0	15,380	454	0	16,572	4,412
Methoxyacetic acid	625-45-6	161	20	9	514	584
N,N-Dimethylformamide	68-12-2	422	36	2	770	2,972
Naphthalene	91-20-3	220	35	0	627	5,945
Nitrogen, liquid	7727-37-9	129,875	82,599	9,594	335,858	713
Ozone	10028-15-6	129	126	71	212	209
Peracetic acid	79-21-0	1,251	1,117	209	2,762	221
Phosphonic acid	13598-36-2	7,730	3	0	18	2,216
Phosphoric acid Divosan X-Tend formulation	7664-38-2	48	14	0	54	315
Potassium acetate	127-08-2	1,216	5	0	5,793	325

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Propargyl alcohol	107-19-7	658	9	0	183	10,771
Saline	7647-14-5	7,197	696	0	12,682	6,673
Saturated sucrose	57-50-1	6	2	0	7	125
Silica, amorphous	7631-86-9	57,267	71	0	319,553	2,423
Sodium carbonate	497-19-8	2,191	158	0	12,678	396
Sodium formate	141-53-7	2	1	1	2	204
Sodium hydroxide	1310-73-2	4,445	306	2	10,701	12,585
Sulfur dioxide	7446-09-5	2	0	0	0	224
Sulfuric acid	7664-93-9	18	0	0	22	402
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	532	218	0	1,898	814
Tetramethylammonium chloride	75-57-0	4,296	2,141	10	15,537	3,162
Thioglycolic acid	68-11-1	277	37	8	1,155	156
Toluene	108-88-3	59	0	0	35	214
Tridecane	629-50-5	541	88	0	541	132
Triethanolamine	102-71-6	3,588	255	0	9,599	1,498
Triethyl phosphate	78-40-0	222	6	0	2,140	991
Triethylene glycol	112-27-6	22,038	491	119	4,008	528
Triisopropanolamine	122-20-3	177	17	4	1,274	251
Trimethyl borate	121-43-7	292	141	14	997	294
Undecane	1120-21-4	766	82	0	4,597	241

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

Table C-7. Associated chemical densities and references used to calculate chemical mass and estimate chemical volume.

Name	CASRN	Density (g/mL)	Reference
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	0.84	Dejoye Tanzi et al. (2012)
1-Butoxy-2-propanol	5131-66-8	0.88	Pal et al. (2013)
1-Decanol	112-30-1	0.83	Faria et al. (2013)
1-Octanol	111-87-5	0.82	Dubey and Kumar (2013)
1-Propanol	71-23-8	0.8	Rani and Maken (2013)
1,2-Propylene glycol	57-55-6	1.03	Moosavi et al. (2013)
1,2,4-Trimethylbenzene	95-63-6	0.87	He et al. (2008)
2-Butoxyethanol	111-76-2	0.9	Dhondge et al. (2010)
2-Ethylhexanol	104-76-7	0.83	Laavi et al. (2012)
2-Mercaptoethanol	60-24-2	0.11	Rawat et al. (1976)
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	2.4	Fels (1900)
Acetic acid	64-19-7	1.04	Chafer et al. (2010)
Acetic anhydride	108-24-7	1.07	Radwan and Hanna (1976)
Acrylamide	79-06-1	1.13	Carpenter and Davis (1957)
Adipic acid	124-04-9	1.36	Thalladi et al. (2000)
Aluminum chloride	7446-70-0	2.44	Sigma-Aldrich (2015a)
Ammonia	7664-41-7	0.67	Harlow et al. (1997)
Ammonium acetate	631-61-8	1.17	Biltz and Balz (1928)
Ammonium chloride	12125-02-9	1.519	Haynes (2014)
Ammonium hydroxide	1336-21-6	1.8	Xiao et al. (2013)
Benzyl chloride	100-44-7	1.09	Sarkar et al. (2012)
Carbonic acid, dipotassium salt	584-08-7	2.43	Sigma-Aldrich (2014b)
Chlorine dioxide	10049-04-4	2.757	Haynes (2014)
Choline chloride	67-48-1	1.17	Shanley and Collin (1961)
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	1.1	Masood et al. (1976)
Citric acid	77-92-9	1.6	Bennett and Yuill (1935)
Dibromoacetonitrile	3252-43-5	2.37	Wilt (1956)
Diethylene glycol	111-46-6	1.12	Chasib (2013)
Diethylenetriamine	111-40-0	0.95	Dubey and Kumar (2011)
Dodecane	112-40-3	0.75	Baragi et al. (2013)

Name	CASRN	Density (g/mL)	Reference
Ethanol	64-17-5	0.79	Kiselev et al. (2012)
Ethanolamine	141-43-5	1.01	Blanco et al. (2013)
Ethyl acetate	141-78-6	0.89	Laavi et al. (2013)
Ethylene glycol	107-21-1	1.1	Rodnikova et al. (2012)
Ferric chloride	7705-08-0	2.9	Haynes (2014)
Formalin	50-00-0	1.08	Alfa Aesar (2015)
Formic acid	64-18-6	1.22	Casanova et al. (1981)
Fumaric acid	110-17-8	1.64	Huffman and Fox (1938)
Glutaraldehyde	111-30-8	1	Oka (1962)
Glycerin, natural	56-81-5	1.26	Egorov et al. (2013)
Glycolic acid	79-14-1	1.49	Pijper (1971)
Hydrochloric acid	7647-01-0	1	Steinhauser et al. (1990)
Isopropanol	67-63-0	0.78	Zhang et al. (2013)
Isopropylamine	75-31-0	0.68	Sarkar and Roy (2009)
Magnesium chloride	7786-30-3	2.32	Haynes (2014)
Methanol	67-56-1	0.79	Kiselev et al. (2012)
Methenamine	100-97-0	1.2	Mak (1965)
Methoxyacetic acid	625-45-6	1.18	Haynes (2014)
N,N-Dimethylformamide	68-12-2	0.94	Smirnov and Badelin (2013)
Naphthalene	91-20-3	0.81	Dyshin et al. (2008)
Nitrogen, liquid	7727-37-9	0.8	finemech (2012)
Ozone	10028-15-6	0.002144	Haynes (2014)
Peracetic acid	79-21-0	1.1	Sigma-Aldrich (2015b)
Phosphonic acid	13598-36-2	1.7	Sigma-Aldrich (2014a)
Phosphoric acid Divosan X-Tend formulation	7664-38-2	0.94	Fadeeva et al. (2004)
Potassium acetate	127-08-2	1.57	Haynes (2014)
Propargyl alcohol	107-19-7	0.95	Vijaya Kumar et al. (1996)
Saline	7647-14-5	2.17	Sigma-Aldrich (2010)
Saturated sucrose	57-50-1	1.13	Hagen and Kaatze (2004)
Silica, amorphous	7631-86-9	2.2	Fujino et al. (2004)
Sodium carbonate	497-19-8	2.54	Haynes (2014)
Sodium formate	141-53-7	1.97	Fuess et al. (1982)

Name	CASRN	Density (g/mL)	Reference
Sodium hydroxide	1310-73-2	2.13	Haynes (2014)
Sulfur dioxide	7446-09-5	1.3	Sigma-Aldrich (2015c)
Sulfuric acid	7664-93-9	1.83	Sigma-Aldrich (2015d)
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	0.9	Sigma-Aldrich (2007)
Tetramethylammonium chloride	75-57-0	1.17	Haynes (2014)
Thioglycolic acid	68-11-1	1.33	Biilmann (1906)
Toluene	108-88-3	0.86	Martinez-Reina et al. (2012)
Tridecane	629-50-5	0.75	Zhang et al. (2011)
Triethanolamine	102-71-6	1.12	Blanco et al. (2013)
Triethyl phosphate	78-40-0	1.06	Krakowiak et al. (2001)
Triethylene glycol	112-27-6	1.12	Afzal et al. (2009)
Triisopropanolamine	122-20-3	1.02	IUPAC (2014)
Trimethyl borate	121-43-7	0.93	Sigma-Aldrich (2015e)
Undecane	1120-21-4	0.74	de Oliveira et al. (2011)

Table C-8. Selected physicochemical properties of chemicals reported as used in hydraulic fracturing fluids.

Properties are provided for chemicals, where available from EPI Suite™ version 4.1 (U.S. EPA, 2012a).

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
(13Z)-N,N-bis(2-hydroxyethyl)-N-methyldocos-13-en-1-aminium chloride	120086-58-0	4.38	--	0.3827	3.32×10^{-15}	--	--
(2,3-Dihydroxypropyl)trimethyl ammonium chloride	34004-36-9	-5.8	--	1.00×10^{6}	9.84×10^{-18}	--	--
(E)-Crotonaldehyde	123-73-9	0.6	--	4.15×10^{4}	5.61×10^{-5}	1.90×10^{-5}	1.94×10^{-5}
[Nitrilotris(methylene)]tris-phosphonic acid pentasodium salt	2235-43-0	−5.45	−3.53	1.00×10^{6}	1.65×10^{-34}	--	--
1-(1-Naphthylmethyl)quinolinium chloride	65322-65-8	5.57	--	0.02454	1.16×10^{-7}	--	--
1-(Alkyl* amino)-3-aminopropane *(42%C12, 26%C18, 15%C14, 8%C16, 5%C10, 4%C8)	68155-37-3	4.74	--	23.71	6.81×10^{-8}	2.39×10^{-8}	--
1-(Phenylmethyl)pyridinium Et Me derivatives, chlorides	68909-18-2	4.1	--	14.13	1.78×10^{-5}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1,2,3-Trimethylbenzene	526-73-8	3.63	3.66	75.03	7.24×10^{-3}	6.58×10^{-3}	4.36×10^{-3}
1,2,4-Trimethylbenzene	95-63-6	3.63	3.63	79.59	7.24×10^{-3}	6.58×10^{-3}	6.16×10^{-3}
1,2-Benzisothiazolin-3-one	2634-33-5	0.64	--	2.14×10^{4}	6.92×10^{-9}	--	--
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	1.63	--	424	3.94×10^{-10}	--	--
1,2-Dimethylbenzene	95-47-6	3.09	3.12	224.1	6.56×10^{-3}	6.14×10^{-3}	5.18×10^{-3}
1,2-Ethanediaminium, N,N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4	−23.19	--	1.00×10^{6}	2.33×10^{-35}	--	--
1,2-Propylene glycol	57-55-6	-0.78	−0.92	8.11×10^{5}	1.74×10^{-7}	1.31×10^{-10}	1.29×10^{-8}
1,2-Propylene oxide	75-56-9	0.37	0.03	1.29×10^{5}	1.60×10^{-4}	1.23×10^{-4}	6.96×10^{-5}
1,3,5-Triazine	290-87-9	−0.2	0.12	1.03×10^{5}	1.21×10^{-6}	--	--
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	−4.67	--	1.00×10^{6}	1.08×10^{-11}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1,3,5-Trimethylbenzene	108-67-8	3.63	3.42	120.3	7.24×10^{-3}	6.58×10^{-3}	8.77×10^{-3}
1,3-Butadiene	106-99-0	2.03	1.99	792.3	7.79×10^{-2}	7.05×10^{-2}	7.36×10^{-2}
1,3-Dichloropropene	542-75-6	2.29	2.04	1,994	2.45×10^{-2}	3.22×10^{-3}	3.55×10^{-3}
1,4-Dioxane	123-91-1	−0.32	−0.27	2.14×10^{5}	5.91×10^{-6}	1.12×10^{-7}	4.80×10^{-6}
1,6-Hexanediamine	124-09-4	0.35	--	5.34×10^{5}	3.21×10^{-9}	7.05×10^{-10}	--
1,6-Hexanediamine dihydrochloride	6055-52-3	0.35	--	5.34×10^{5}	3.21×10^{-9}	7.05×10^{-10}	--
1-[2-(2-Methoxy-1-methylethoxy)-1-methylethoxy]-2-propanol	20324-33-8	−0.2	--	1.96×10^{5}	2.36×10^{-11}	4.55×10^{-13}	--
1-Amino-2-propanol	78-96-6	−1.19	−0.96	1.00×10^{6}	4.88×10^{-10}	2.34×10^{-10}	--
1-Benzylquinolinium chloride	15619-48-4	4.4	--	6.02	1.19×10^{-6}	--	--
1-Butanol	71-36-3	0.84	0.88	7.67×10^{4}	9.99×10^{-6}	9.74×10^{-6}	8.81×10^{-6}
1-Butoxy-2-propanol	5131-66-8	0.98	--	4.21×10^{4}	1.30×10^{-7}	4.88×10^{-8}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Decanol	112-30-1	3.79	4.57	28.21	5.47×10^{-5}	7.73×10^{-5}	3.20×10^{-5}
1-Dodecyl-2-pyrrolidinone	2687-96-9	5.3	4.2	5.862	7.12×10^{-7}	--	--
1-Eicosene	3452-07-1	10.03	--	1.26×10^{-5}	1.89×10^{1}	6.74×10^{1}	--
1-Ethyl-2-methylbenzene	611-14-3	3.58	3.53	96.88	8.71×10^{-3}	9.52×10^{-3}	5.53×10^{-3}
1-Hexadecene	629-73-2	8.06	--	0.001232	6.10	1.69×10^{1}	--
1-Hexanol	111-27-3	1.82	2.03	6,885	1.76×10^{-5}	1.94×10^{-5}	1.71×10^{-5}
1-Methoxy-2-propanol	107-98-2	−0.49	--	1.00×10^{6}	5.56×10^{-8}	1.81×10^{-8}	9.20×10^{-7}
1-Octadecanamine, acetate (1:1)	2190-04-7	7.71	--	0.04875	9.36×10^{-4}	2.18×10^{-3}	--
1-Octadecanamine, N,N-dimethyl-	124-28-7	8.39	--	0.008882	4.51×10^{-3}	3.88×10^{-2}	--
1-Octadecene	112-88-9	9.04	--	1.256×10^{-4}	10.7	3.38×10^{1}	--
1-Octanol	111-87-5	2.81	3	814	3.10×10^{-5}	3.88×10^{-5}	2.45×10^{-5}
1-Pentanol	71-41-0	1.33	1.51	2.09×10^{4}	1.33×10^{-5}	1.38×10^{-5}	1.30×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3327-22-8	−4.48	--	1.00×10^{6}	9.48×10^{-17}	--	--
1-Propanesulfonic acid	5284-66-2	−1.4	--	1.00×10^{6}	2.22×10^{-8}	--	--
1-Propanol	71-23-8	0.35	0.25	2.72×10^{5}	7.52×10^{-6}	6.89×10^{-6}	7.41×10^{-6}
1-Propene	115-07-1	1.68	1.77	1,162	1.53×10^{-1}	1.58×10^{-1}	1.96×10^{-1}
1-tert-Butoxy-2-propanol	57018-52-7	0.87	--	5.24×10^{4}	1.30×10^{-7}	5.23×10^{-8}	--
1-Tetradecene	1120-36-1	7.08	--	0.01191	3.46	8.48	--
1-Tridecanol	112-70-9	5.26	--	4.533	1.28×10^{-4}	2.18×10^{-4}	--
1-Undecanol	112-42-5	4.28	--	43.04	7.26×10^{-5}	1.09×10^{-4}	--
2-(2-Butoxyethoxy)ethanol	112-34-5	0.29	0.56	7.19×10^{4}	1.52×10^{-9}	4.45×10^{-11}	7.20×10^{-9}
2-(2-Ethoxyethoxy)ethanol	111-90-0	−0.69	−0.54	8.28×10^{5}	8.63×10^{-10}	2.23×10^{-11}	2.23×10^{-8}
2-(2-Ethoxyethoxy)ethyl acetate	112-15-2	0.32	--	3.09×10^{4}	5.62×10^{-8}	7.22×10^{-10}	2.29×10^{-8}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-(Dibutylamino)ethanol	102-81-8	2.01	2.65	3,297	9.70×10^{-9}	1.02×10^{-8}	--
2-(Hydroxymethylamino)ethanol	34375-28-5	−1.53	--	1.00×10^{6}	1.62×10^{-12}	--	--
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	3.12	3.3	41.67	6.49×10^{-12}	--	--
2,2'-(Diazene-1,2-diyldiethane-1,1-diyl)bis-4,5-dihydro-1H-imidazole dihydrochloride	27776-21-2	2.12	--	193.3	3.11×10^{-14}	--	--
2,2'-(Octadecylimino)diethanol	10213-78-2	6.85	--	0.08076	1.06×10^{-8}	7.39×10^{-12}	--
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	−2.17	--	1.00×10^{6}	2.50×10^{-13}	8.10×10^{-16}	--
2,2'-Azobis(2-amidinopropane) dihydrochloride	2997-92-4	−3.28	--	1.00×10^{6}	1.21×10^{-14}	--	--
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1.01	0.82	2,841	6.16×10^{-14}	--	1.91×10^{-8}
2,2-Dibromopropanediamide	73003-80-2	0.37	--	1.00×10^{4}	3.58×10^{-14}	--	--
2,4-Hexadienoic acid, potassium salt, (2E,4E)-	24634-61-5	1.62	1.33	1.94×10^{4}	5.72×10^{-7}	4.99×10^{-8}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2,6,8-Trimethyl-4-nonanol	123-17-1	4.48	--	24.97	9.63×10^{-5}	4.45×10^{-4}	--
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	−2.19	--	1.00×10^{6}	5.18×10^{-15}	--	--
2-Amino-2-methylpropan-1-ol	124-68-5	−0.74	--	1.00×10^{6}	6.48×10^{-10}	--	--
2-Aminoethanol hydrochloride	2002-24-6	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
2-Bromo-3-nitrilopropionamide	1113-55-9	−0.31	--	3,274	5.35×10^{-13}	--	--
2-Butanone oxime	96-29-7	1.69	0.63	3.66×10^{4}	1.04×10^{-5}	--	--
2-Butoxy-1-propanol	15821-83-7	0.98	--	4.21×10^{4}	1.30×10^{-7}	4.88×10^{-8}	--
2-Butoxyethanol	111-76-2	0.57	0.83	6.45×10^{4}	9.79×10^{-8}	2.08×10^{-8}	1.60×10^{-6}
2-Dodecylbenzenesulfonic acid- N-(2-aminoethyl)ethane-1,2-diamine(1:1)	40139-72-8	4.78	--	0.7032	6.27×10^{-8}	--	--
2-Ethoxyethanol	110-80-5	−0.42	−0.32	7.55×10^{5}	5.56×10^{-8}	1.04×10^{-8}	4.70×10^{-7}
2-Ethoxynaphthalene	93-18-5	3.74	--	38.32	4.13×10^{-5}	4.06×10^{-4}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-Ethyl-1-hexanol	104-76-7	2.73	--	1,379	3.10×10^{-5}	4.66×10^{-5}	2.65×10^{-5}
2-Ethyl-2-hexenal	645-62-5	2.62	--	548.6	2.06×10^{-4}	4.88×10^{-4}	--
2-Ethylhexyl benzoate	5444-75-7	5.19	--	1.061	2.52×10^{-4}	2.34×10^{-4}	--
2-Hydroxyethyl acrylate	818-61-1	−0.25	−0.21	5.07×10^{5}	4.49×10^{-9}	7.22×10^{-10}	--
2-Hydroxyethylammonium hydrogen sulphite	13427-63-9	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	7006-59-9	−6.7	--	1.00×10^{6}	4.78×10^{-19}	--	--
2-Mercaptoethanol	60-24-2	−0.2	--	1.94×10^{5}	1.27×10^{-7}	3.38×10^{-8}	1.80×10^{-7}
2-Methoxyethanol	109-86-4	−0.91	−0.77	1.00×10^{6}	4.19×10^{-8}	7.73×10^{-9}	3.30×10^{-7}
2-Methyl-1-propanol	78-83-1	0.77	0.76	9.71×10^{4}	9.99×10^{-6}	1.17×10^{-5}	9.78×10^{-6}
2-Methyl-2,4-pentanediol	107-41-5	0.58	--	3.26×10^{4}	4.06×10^{-7}	3.97×10^{-10}	--
2-Methyl-3(2H)-isothiazolone	2682-20-4	−0.83	--	5.37×10^{5}	4.96×10^{-8}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
2-Methyl-3-butyn-2-ol	115-19-5	0.45	0.28	2.40×10^{5}	1.04×10^{-6}	--	3.91×10^{-6}
2-Methylbutane	78-78-4	2.72	--	184.6	1.29	1.44	1.40
2-Methylquinoline hydrochloride	62763-89-7	2.69	2.59	498.5	7.60×10^{-7}	2.13×10^{-6}	--
2-Phosphono-1,2,4-butanetricarboxylic acid	37971-36-1	−1.66	--	1.00×10^{6}	1.17×10^{-26}	--	--
2-Phosphonobutane-1,2,4-tricarboxylic acid, potassium salt (1:x)	93858-78-7	−1.66	--	1.00×10^{6}	1.17×10^{-26}	--	--
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	13533-05-6	−0.52	−0.3	3.99×10^{5}	6.98×10^{-11}	1.54×10^{-12}	--
3-(Dimethylamino)propylamine	109-55-7	−0.45	--	1.00×10^{6}	6.62×10^{-9}	4.45×10^{-9}	--
3,4,4-Trimethyloxazolidine	75673-43-7	0.13	--	8.22×10^{5}	6.63×10^{-6}	--	--
3,5,7-Triazatricyclo(3.3.1.13,7))decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-	51229-78-8	−5.92	--	1.00×10^{6}	1.76×10^{-8}	--	--
3,7-Dimethyl-2,6-octadienal	5392-40-5	3.45	--	84.71	3.76×10^{-4}	4.35×10^{-5}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
3-Hydroxybutanal	107-89-1	−0.72	--	1.00×10^{6}	4.37×10^{-9}	2.28×10^{-9}	--
3-Methoxypropylamine	5332-73-0	−0.42	--	1.00×10^{6}	1.56×10^{-7}	1.94×10^{-8}	--
3-Phenylprop-2-enal	104-55-2	1.82	1.9	2,150	1.60×10^{-6}	3.38×10^{-7}	--
4,4-Dimethyloxazolidine	51200-87-4	−0.08	--	1.00×10^{6}	3.02×10^{-6}	--	--
4,6-Dimethyl-2-heptanone	19549-80-5	2.56	--	528.8	2.71×10^{-4}	4.55×10^{-4}	--
4-[Abieta-8,11,13-trien-18-yl(3-oxo-3-phenylpropyl)amino]butan-2-one hydrochloride	143106-84-7	7.72	--	0.002229	2.49×10^{-12}	1.20×10^{-14}	--
4-Ethyloct-1-yn-3-ol	5877-42-9	2.87	--	833.9	4.27×10^{-6}	--	--
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	1.05	1.21	6,875	8.27×10^{-11}	2.81×10^{-9}	2.15×10^{-9}
4-Methoxybenzyl formate	122-91-8	1.61	--	2,679	1.15×10^{-6}	2.13×10^{-6}	--
4-Methoxyphenol	150-76-5	1.59	1.58	1.65×10^{4}	3.32×10^{-8}	5.35×10^{-7}	--
4-Methyl-2-pentanol	108-11-2	1.68	--	1.38×10^{4}	1.76×10^{-5}	3.88×10^{-5}	4.45×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
4-Methyl-2-pentanone	108-10-1	1.16	1.31	8,888	1.16×10^{-4}	1.34×10^{-4}	1.38×10^{-4}
4-Nonylphenol	104-40-5	5.99	5.76	1.57	5.97×10^{-6}	1.23×10^{-5}	3.40×10^{-5}
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	−0.34	--	1.49×10^{5}	3.57×10^{-8}	--	--
Acetaldehyde	75-07-0	−0.17	−0.34	2.57×10^{5}	6.78×10^{-5}	6.00×10^{-5}	6.67×10^{-5}
Acetic acid	64-19-7	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Acetic acid, C6-8-branched alkyl esters	90438-79-2	3.25	--	117.8	9.60×10^{-4}	1.07×10^{-3}	--
Acetic acid, hydroxy-, reaction products with triethanolamine	68442-62-6	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}
Acetic acid, mercapto-, monoammonium salt	5421-46-5	0.03	0.09	2.56×10^{5}	1.94×10^{-8}	--	--
Acetic anhydride	108-24-7	−0.58	--	3.59×10^{5}	3.57×10^{-5}	--	5.71×10^{-6}
Acetone	67-64-1	−0.24	−0.24	2.20×10^{5}	4.96×10^{-5}	3.97×10^{-5}	3.50×10^{-5}
Acetonitrile, 2,2',2''-nitrilotris-	7327-60-8	−1.39	--	1.00×10^{6}	2.61×10^{-15}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Acetophenone	98-86-2	1.67	1.58	4,484	9.81×10^{-6}	1.09×10^{-5}	1.04×10^{-5}
Acetyltriethyl citrate	77-89-4	1.34	--	688.2	6.91×10^{-11}	--	--
Acrolein	107-02-8	0.19	−0.01	1.40×10^{5}	3.58×10^{-5}	1.94×10^{-5}	1.22×10^{-4}
Acrylamide	79-06-1	−0.81	−0.67	5.04×10^{5}	5.90×10^{-9}	--	1.70×10^{-9}
Acrylic acid	79-10-7	0.44	0.35	1.68×10^{5}	2.89×10^{-7}	1.17×10^{-7}	3.70×10^{-7}
Acrylic acid, with sodium-2-acrylamido-2-methyl-1-propanesulfonate and sodium phosphinate	110224-99-2	−2.19	--	1.00×10^{6}	5.18×10^{-15}	--	--
Alcohols, C10-12, ethoxylated	67254-71-1	5.47	--	0.9301	1.95×10^{-2}	2.03×10^{-2}	--
Alcohols, C11-14-iso-, C13-rich	68526-86-3	5.19	--	5.237	1.28×10^{-4}	2.62×10^{-4}	--
Alcohols, C11-14-iso-, C13-rich, ethoxylated	78330-21-9	4.91	--	5.237	1.25×10^{-6}	7.73×10^{-7}	--
Alcohols, C12-13, ethoxylated	66455-14-9	5.96	--	0.2995	2.58×10^{-2}	2.87×10^{-2}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Alcohols, C12-14, ethoxylated propoxylated	68439-51-0	6.67	--	0.02971	7.08×10^{-4}	1.23×10^{-4}	--
Alcohols, C12-14-secondary	126950-60-5	5.19	--	5.237	1.28×10^{-4}	3.62×10^{-4}	--
Alcohols, C12-16, ethoxylated	68551-12-2	6.45	--	0.09603	3.43×10^{-2}	4.06×10^{-2}	--
Alcohols, C14-15, ethoxylated	68951-67-7	7.43	--	0.009765	6.04×10^{-2}	8.10×10^{-2}	--
Alcohols, C6-12, ethoxylated	68439-45-2	4.49	--	8.832	1.10×10^{-2}	1.02×10^{-2}	--
Alcohols, C7-9-iso-, C8-rich, ethoxylated	78330-19-5	2.46	--	1,513	3.04×10^{-7}	1.38×10^{-7}	--
Alcohols, C9-11, ethoxylated	68439-46-3	4.98	--	2.874	1.47×10^{-2}	1.44×10^{-2}	--
Alcohols, C9-11-iso-, C10-rich, ethoxylated	78330-20-8	4.9	--	3.321	1.47×10^{-2}	2.39×10^{-2}	--
Alkanes, C12-14-iso-	68551-19-9	6.65	--	0.03173	1.24×10^{1}	2.28×10^{1}	--
Alkanes, C13-16-iso-	68551-20-2	7.63	--	0.003311	2.19×10^{1}	4.55×10^{1}	--
Alkenes, C>10 alpha-	64743-02-8	8.55	--	0.0003941	8.09	2.39×10^{1}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Alkyl* dimethyl ethylbenzyl ammonium chloride *(50%C12, 30%C14, 17%C16, 3%C18)	85409-23-0_1	3.97	--	3.23	1.11×10^{-11}	--	--
Alkyl* dimethyl ethylbenzyl ammonium chloride *(60%C14, 30%C16, 5%C12, 5%C18)	68956-79-6	4.95	--	0.3172	1.96×10^{-11}	--	--
Alkylbenzenesulfonate, linear	42615-29-2	4.71	--	0.8126	6.27×10^{-8}	--	--
alpha-Lactose monohydrate	5989-81-1	−5.12	--	1.00×10^{6}	4.47×10^{-22}	9.81×10^{-45}	--
alpha-Terpineol	98-55-5	3.33	2.98	371.7	1.58×10^{-5}	3.15×10^{-6}	1.22×10^{-5}
Amaranth	915-67-3	1.63	--	1.789	1.49×10^{-30}	--	--
Aminotrimethylene phosphonic acid	6419-19-8	−5.45	−3.53	1.00×10^{6}	1.65×10^{-34}	--	--
Ammonium acetate	631-61-8	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Ammonium acrylate	10604-69-0	0.44	0.35	1.68×10^{5}	2.89×10^{-7}	1.17×10^{-7}	3.70×10^{-7}
Ammonium citrate (1:1)	7632-50-0	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ammonium citrate (2:1)	3012-65-5	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Ammonium dodecyl sulfate	2235-54-3	2.42	--	163.7	1.84×10^{-7}	--	--
Ammonium hydrogen carbonate	1066-33-7	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Ammonium lactate	515-98-0	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Anethole	104-46-1	3.39	--	98.68	2.56×10^{-4}	2.23×10^{-3}	--
Aniline	62-53-3	1.08	0.9	2.08×10^{4}	1.90×10^{-6}	2.18×10^{-6}	2.02×10^{-6}
Benactyzine hydrochloride	57-37-4	2.89	--	292.1	2.07×10^{-10}	--	--
Benzamorf	12068-08-5	4.71	--	0.8126	6.27×10^{-8}	--	--
Benzene	71-43-2	1.99	2.13	2,000	5.39×10^{-3}	5.35×10^{-3}	5.55×10^{-3}
Benzene, C10-16-alkyl derivatives	68648-87-3	8.43	9.36	0.0002099	1.78×10^{-1}	3.97×10^{-1}	--
Benzenesulfonic acid	98-11-3	−1.17	--	6.90×10^{5}	2.52×10^{-9}	--	--
Benzenesulfonic acid, (1-methylethyl)-,	37953-05-2	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Benzenesulfonic acid, (1-methylethyl)-, ammonium salt	37475-88-0	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--
Benzenesulfonic acid, (1-methylethyl)-, sodium salt	28348-53-0	0.29	--	2.46×10^{4}	4.89×10^{-9}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with cyclohexylamine	255043-08-4	4.71	--	0.8126	6.27×10^{-8}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with triethanolamine	68584-25-8	5.2	--	0.255	8.32×10^{-8}	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, potassium salts	68584-27-0	5.2	--	0.255	8.32×10^{-8}	--	--
Benzenesulfonic acid, dodecyl-, branched, compounds with 2-propanamine	90218-35-2	4.49	--	1.254	6.27×10^{-8}	--	--
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, sodium salts	68081-81-2	4.22	--	2.584	4.72×10^{-8}	--	--
Benzoic acid	65-85-0	1.87	1.87	2,493	1.08×10^{-7}	4.55×10^{-8}	3.81×10^{-8}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Benzyl chloride	100-44-7	2.79	2.3	1,030	2.09×10^{-3}	3.97×10^{-4}	4.12×10^{-4}
Benzyldimethyldodecylammonium chloride	139-07-1	2.93	--	36.47	7.61×10^{-12}	--	--
Benzylhexadecyldimethylammonium chloride	122-18-9	4.89	--	0.3543	2.36×10^{-11}	--	--
Benzyltrimethylammonium chloride	56-93-9	−2.47	--	1.00×10^{6}	3.37×10^{-13}	--	--
Bicine	150-25-4	−3.27	--	3.52×10^{5}	1.28×10^{-14}	--	--
Bis(1-methylethyl)naphthalenesulfonic acid, cyclohexylamine salt	68425-61-6	2.92	--	43.36	9.29×10^{-10}	--	--
Bis(2-chloroethyl) ether	111-44-4	1.56	1.29	6,435	1.89×10^{-4}	4.15×10^{-7}	1.70×10^{-5}
Bisphenol A	80-05-7	3.64	3.32	172.7	9.16×10^{-12}	--	--
Bronopol	52-51-7	−1.51	--	8.37×10^{5}	6.35×10^{-21}	--	--
Butane	106-97-8	2.31	2.89	135.6	9.69×10^{-1}	8.48×10^{-1}	9.50×10^{-1}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	2373-38-8	3.98	--	0.1733	1.61×10^{-12}	--	--
Butene	25167-67-3	2.17	2.4	354.8	2.03×10^{-1}	2.68×10^{-1}	2.33×10^{-1}
Butyl glycidyl ether	2426-08-6	1.08	0.63	2.66×10^{4}	4.37×10^{-6}	5.23×10^{-7}	2.47×10^{-5}
Butyl lactate	138-22-7	0.8	--	5.30×10^{4}	8.49×10^{-5}	--	1.92×10^{-6}
Butyryl trihexyl citrate	82469-79-2	8.21	--	5.56×10^{-5}	3.65×10^{-9}	--	--
C.I. Acid Red 1	3734-67-6	0.51	--	6.157	3.73×10^{-29}	--	--
C.I. Acid Violet 12, disodium salt	6625-46-3	0.59	--	3.379	2.21×10^{-30}	--	--
C.I. Pigment Red 5	6410-41-9	7.65	--	4.38×10^{-5}	4.36×10^{-21}	--	--
C.I. Solvent Red 26	4477-79-6	9.27	--	5.68×10^{-5}	5.48×10^{-13}	4.66×10^{-13}	--
C10-16-Alkyldimethylamines oxides	70592-80-2	2.87	--	89.63	1.14×10^{-13}	--	--
C10-C16 Ethoxylated alcohol	68002-97-1	4.99	--	4.532	1.25×10^{-6}	4.66×10^{-7}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
C12-14 tert-Alkyl ethoxylated amines	73138-27-9	3.4	--	264.2	1.29×10^{-10}	--	--
Calcium dodecylbenzene sulfonate	26264-06-2	4.71	--	0.8126	6.27×10^{-8}	--	--
Camphor	76-22-2	3.04	2.38	339.1	7.00×10^{-5}	--	8.10×10^{-5}
Carbon dioxide	124-38-9	0.83	0.83	2.57×10^{4}	1.52×10^{-2}	--	1.52×10^{-2}
Carbonic acid, dipotassium salt	584-08-7	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Choline bicarbonate	78-73-9	−5.16	--	1.00×10^{6}	2.03×10^{-16}	--	--
Choline chloride	67-48-1	−5.16	--	1.00×10^{6}	2.03×10^{-16}	--	--
Citric acid	77-92-9	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Citronellol	106-22-9	3.56	3.91	105.5	5.68×10^{-5}	2.13×10^{-5}	--
Coconut trimethylammonium chloride	61789-18-2	1.22	--	2,816	9.42×10^{-11}	--	--
Coumarin	91-64-5	1.51	1.39	5,126	6.95×10^{-6}	--	9.92×10^{-8}
Cumene	98-82-8	3.45	3.66	75.03	1.05×10^{-2}	1.23×10^{-2}	1.15×10^{-2}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Cyclohexane	110-82-7	3.18	3.44	43.02	2.55×10^{-1}	1.94×10^{-1}	1.50×10^{-1}
Cyclohexanol	108-93-0	1.64	1.23	3.37×10^{4}	4.90×10^{-6}	3.70×10^{-6}	4.40×10^{-6}
Cyclohexanone	108-94-1	1.13	0.81	2.41×10^{4}	5.11×10^{-5}	1.28×10^{-5}	9.00×10^{-6}
Cyclohexylamine sulfate	19834-02-7	1.63	1.49	6.40×10^{4}	1.38×10^{-5}	--	4.16×10^{-6}
D&C Red no. 28	18472-87-2	9.62	--	1.64×10^{-8}	6.37×10^{-21}	--	--
D&C Red no. 33	3567-66-6	0.48	--	11.87	1.15×10^{-26}	--	--
Daidzein	486-66-8	2.55	--	568.4	3.91×10^{-16}	--	--
Dapsone	80-08-0	0.77	0.97	3,589	3.11×10^{-14}	--	--
Dazomet	533-74-4	0.94	0.63	1.94×10^{4}	2.84×10^{-3}	--	4.98×10^{-10}
Decyldimethylamine	1120-24-7	4.46	--	82.23	4.68×10^{-4}	2.45×10^{-3}	--
D-Glucitol	50-70-4	−3.01	−2.2	1.00×10^{6}	7.26×10^{-13}	2.94×10^{-29}	--
D-Gluconic acid	526-95-4	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
D-Glucopyranoside, methyl	3149-68-6	−2.5	--	1.00×10^{6}	1.56×10^{-14}	2.23×10^{-24}	--
D-Glucose	50-99-7	−2.89	−3.24	1.00×10^{6}	9.72×10^{-15}	1.62×10^{-26}	--
Di(2-ethylhexyl) phthalate	117-81-7	8.39	7.6	0.001132	1.18×10^{-5}	1.02×10^{-5}	2.70×10^{-7}
Dibromoacetonitrile	3252-43-5	0.47	--	9,600	4.06×10^{-7}	--	--
Dichloromethane	75-09-2	1.34	1.25	1.10×10^{4}	9.14×10^{-3}	3.01×10^{-3}	3.25×10^{-3}
Didecyldimethylammonium chloride	7173-51-5	4.66	--	0.9	6.85×10^{-10}	--	--
Diethanolamine	111-42-2	−1.71	−1.43	1.00×10^{6}	3.92×10^{-11}	3.46×10^{-15}	3.87×10^{-11}
Diethylbenzene	25340-17-4	4.07	3.72	58.86	1.16×10^{-2}	1.47×10^{-2}	2.61×10^{-3}
Diethylene glycol	111-46-6	−1.47	--	1.00×10^{6}	2.03×10^{-9}	1.20×10^{-13}	--
Diethylene glycol monomethyl ether	111-77-3	−1.18	--	1.00×10^{6}	6.50×10^{-10}	1.65×10^{-11}	--
Diethylenetriamine	111-40-0	−2.13	--	1.00×10^{6}	3.10×10^{-13}	1.09×10^{-14}	--
Diisobutyl ketone	108-83-8	2.56	--	528.8	2.71×10^{-4}	4.55×10^{-4}	1.17×10^{-4}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Diisopropanolamine	110-97-4	−0.88	−0.82	1.00×10^{6}	6.91×10^{-11}	1.90×10^{-14}	--
Diisopropylnaphthalene	38640-62-9	6.08	--	0.2421	1.99×10^{-3}	1.94×10^{-3}	--
Dimethyl adipate	627-93-0	1.39	1.03	7,749	9.77×10^{-7}	1.28×10^{-7}	2.31×10^{-6}
Dimethyl glutarate	1119-40-0	0.9	0.62	2.02×10^{4}	7.36×10^{-7}	9.09×10^{-8}	6.43×10^{-7}
Dimethyl succinate	106-65-0	0.4	0.35	3.96×10^{4}	5.54×10^{-7}	6.43×10^{-8}	--
Dimethylaminoethanol	108-01-0	−0.94	--	1.00×10^{6}	1.77×10^{-9}	1.77×10^{-9}	3.73×10^{-7}
Dimethyldiallylammonium chloride	7398-69-8	−2.49	--	1.00×10^{6}	7.20×10^{-12}	--	--
Diphenyl oxide	101-84-8	4.05	4.21	15.58	1.18×10^{-4}	2.81×10^{-4}	2.79×10^{-4}
Dipropylene glycol	25265-71-8	−0.64	--	3.11×10^{5}	3.58×10^{-9}	6.29×10^{-10}	--
Di-sec-butylphenol	31291-60-8	5.41	--	3.723	3.74×10^{-6}	6.89×10^{-6}	--
Disodium dodecyl(sulphonatophenoxy)benzenesulphonate	28519-02-0	5.05	--	0.0353	6.40×10^{-16}	--	--

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Disodium ethylenediaminediacetate	38011-25-5	−4.79	--	1.00×10^{6}	1.10×10^{-16}	--	--
Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
D-Lactic acid	10326-41-7	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
D-Limonene	5989-27-5	4.83	4.57	4.581	3.80×10^{-1}	--	3.19×10^{-2}
Docusate sodium	577-11-7	6.1	--	0.001227	5.00×10^{-12}	--	--
Dodecane	112-40-3	6.23	6.1	0.1099	9.35	1.34×10^{1}	8.18
Dodecylbenzene	123-01-3	7.94	8.65	0.001015	1.34×10^{-1}	2.81×10^{-1}	--
Dodecylbenzenesulfonic acid	27176-87-0	4.71	--	0.8126	6.27×10^{-8}	--	--
Dodecylbenzenesulfonic acid, monoethanolamine salt	26836-07-7	4.71	--	0.8126	6.27×10^{-8}	--	--
Epichlorohydrin	106-89-8	0.63	0.45	5.06×10^{4}	5.62×10^{-5}	2.62×10^{-6}	3.04×10^{-5}

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	44992-01-0	−3.1	--	1.00×10^{6}	6.96×10^{-15}	--	--
Ethane	74-84-0	1.32	1.81	938.6	5.50×10^{-1}	4.25×10^{-1}	5.00×10^{-1}
Ethanol	64-17-5	−0.14	−0.31	7.92×10^{5}	5.67×10^{-6}	4.88×10^{-6}	5.00×10^{-6}
Ethanol, 2,2',2''-nitrilotris-, tris(dihydrogen phosphate) (ester), sodium salt	68171-29-9	−3.13	--	1.00×10^{6}	3.08×10^{-36}	--	--
Ethanol, 2-[2-[2-(tridecyloxy) ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	25446-78-0	2.09	--	42	9.15×10^{-13}	--	--
Ethanolamine	141-43-5	−1.61	−1.31	1.00×10^{6}	3.68×10^{-10}	9.96×10^{-11}	--
Ethoxylated dodecyl alcohol	9002-92-0	4.5	--	14.19	9.45×10^{-7}	3.30×10^{-7}	--
Ethyl acetate	141-78-6	0.86	0.73	2.99×10^{4}	2.33×10^{-4}	1.58×10^{-4}	1.34×10^{-4}
Ethyl acetoacetate	141-97-9	−0.2	0.25	5.62×10^{4}	1.57×10^{-7}	--	1.20×10^{-6}
Ethyl benzoate	93-89-0	2.32	2.64	421.5	4.61×10^{-5}	2.45×10^{-5}	7.33×10^{-5}

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Ethyl lactate	97-64-3	−0.18	--	4.73×10^{5}	4.82×10^{-5}	--	5.83×10^{-7}
Ethyl salicylate	118-61-6	3.09	2.95	737.1	6.04×10^{-6}	3.01×10^{-9}	--
Ethylbenzene	100-41-4	3.03	3.15	228.6	7.89×10^{-3}	8.88×10^{-3}	7.88×10^{-3}
Ethylene	74-85-1	1.27	1.13	3,449	9.78×10^{-2}	1.62×10^{-1}	2.28×10^{-1}
Ethylene glycol	107-21-1	−1.2	−1.36	1.00×10^{6}	1.31×10^{-7}	5.60×10^{-11}	6.00×10^{-8}
Ethylene oxide	75-21-8	−0.05	−0.3	2.37×10^{5}	1.20×10^{-4}	5.23×10^{-5}	1.48×10^{-4}
Ethylenediamine	107-15-3	−1.62	−2.04	1.00×10^{6}	1.03×10^{-9}	1.77×10^{-10}	1.73×10^{-9}
Ethylenediaminetetraacetic acid	60-00-4	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethylenediaminetetraacetic acid, disodium salt	139-33-3	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Ethyne	74-86-2	0.5	0.37	1.48×10^{4}	2.40×10^{-2}	2.45×10^{-2}	2.17×10^{-2}

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		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Fatty acids, C18-unsaturated, dimers	61788-89-4	14.6	--	2.31×10^{-10}	4.12×10^{-8}	9.74×10^{-9}	--
FD&C Blue no. 1	3844-45-9	−0.15	--	0.2205	2.25×10^{-35}	--	--
FD&C Yellow no. 5	1934-21-0	−1.82	--	7.388	1.31×10^{-28}	--	--
FD&C Yellow no. 6	2783-94-0	1.4	--	242.7	3.26×10^{-23}	--	--
Formaldehyde	50-00-0	0.35	0.35	5.70×10^{4}	9.29×10^{-5}	6.14×10^{-5}	3.37×10^{-7}
Formamide	75-12-7	−1.61	−1.51	1.00×10^{6}	1.53×10^{-8}	--	1.39×10^{-9}
Formic acid	64-18-6	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Formic acid, potassium salt	590-29-4	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Fumaric acid	110-17-8	0.05	−0.48	1.04×10^{5}	1.35×10^{-12}	8.48×10^{-14}	--
Furfural	98-01-1	0.83	0.41	5.36×10^{4}	1.34×10^{-5}	--	3.77×10^{-6}
Furfuryl alcohol	98-00-0	0.45	0.28	2.21×10^{5}	2.17×10^{-7}	--	7.86×10^{-8}
Galantamine hydrobromide	69353-21-5	2.29	--	1,606	1.70×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Gluconic acid	133-42-6	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--
Glutaraldehyde	111-30-8	−0.18	--	1.67×10^{5}	1.10×10^{-7}	2.39×10^{-8}	--
Glycerol	56-81-5	−1.65	−1.76	1.00×10^{6}	6.35×10^{-9}	1.51×10^{-15}	1.73×10^{-8}
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	135-37-5	−3.04	--	1.90×10^{5}	3.90×10^{-17}	--	--
Glycine, N-(hydroxymethyl)-, monosodium salt	70161-44-3	−3.41	--	7.82×10^{5}	1.80×10^{-12}	--	--
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	5064-31-3	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--
Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)-, trisodium salt	139-89-9	−4.09	--	4.31×10^{5}	3.81×10^{-24}	--	--
Glycolic acid	79-14-1	−1.07	−1.11	1.00×10^{6}	8.54×10^{-8}	6.29×10^{-11}	--
Glycolic acid sodium salt	2836-32-0	−1.07	−1.11	1.00×10^{6}	8.54×10^{-8}	6.29×10^{-11}	--
Glyoxal	107-22-2	−1.66	--	1.00×10^{6}	3.70×10^{-7}	--	3.33×10^{-9}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Glyoxylic acid	298-12-4	−1.4	--	1.00×10^{6}	2.98×10^{-9}	--	--
Heptane	142-82-5	3.78	4.66	3.554	2.27	2.39	2.00
Hexadecyltrimethylammonium bromide	57-09-0	3.18	--	28.77	2.93×10^{-10}	--	--
Hexane	110-54-3	3.29	3.9	17.24	1.71	1.69	1.80
Hexanedioic acid	124-04-9	0.23	0.08	1.67×10^{5}	9.53×10^{-12}	8.10×10^{-13}	4.71×10^{-12}
Hydroxyvalerenic acid	1619-16-5	3.31	--	282.1	--	--	--
Indole	120-72-9	2.05	2.14	1,529	8.86×10^{-7}	1.99×10^{-6}	5.28×10^{-7}
Isoascorbic acid	89-65-6	−1.88	−1.85	1.00×10^{6}	4.07×10^{-8}	--	--
Isobutane	75-28-5	2.23	2.76	175.1	9.69×10^{-1}	1.02	1.19
Isobutene	115-11-7	2.23	2.34	399.2	2.40×10^{-1}	2.34×10^{-1}	2.18×10^{-1}
Isooctanol	26952-21-6	2.73	--	1,379	3.10×10^{-5}	4.66×10^{-5}	9.21×10^{-5}
Isopentyl alcohol	123-51-3	1.26	1.16	4.16×10^{4}	1.33×10^{-5}	1.65×10^{-5}	1.41×10^{-5}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Isopropanol	67-63-0	0.28	0.05	4.02×10^{5}	7.52×10^{-6}	1.14×10^{-5}	8.10×10^{-6}
Isopropanolamine dodecylbenzene	42504-46-1	7.94	8.65	0.001015	1.34×10^{-1}	2.81×10^{-1}	--
Isopropylamine	75-31-0	0.27	0.26	8.38×10^{5}	1.34×10^{-5}	--	4.51×10^{-5}
Isoquinoline	119-65-3	2.14	2.08	1,551	6.88×10^{-7}	4.15×10^{-7}	--
Isoquinoline, reaction products with benzyl chloride and quinoline	68909-80-8	2.14	2.08	1,551	6.88×10^{-7}	4.15×10^{-7}	--
Isoquinolinium, 2-(phenylmethyl)-, chloride	35674-56-7	4.4	--	6.02	1.19×10^{-6}	--	--
Lactic acid	50-21-5	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Lactose	63-42-3	−5.12	--	1.00×10^{6}	4.47×10^{-22}	9.81×10^{-45}	--
Lauryl hydroxysultaine	13197-76-7	−1.3	--	7.71×10^{4}	1.04×10^{-21}	--	--
L-Dilactide	4511-42-6	1.65	--	3,165	1.22×10^{-5}	--	--
L-Glutamic acid	56-86-0	−3.83	−3.69	9.42×10^{5}	1.47×10^{-14}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
L-Lactic acid	79-33-4	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Methane	74-82-8	0.78	1.09	2,610	4.14×10^{-1}	6.58×10^{-1}	6.58×10^{-1}
Methanol	67-56-1	−0.63	−0.77	1.00×10^{6}	4.27×10^{-6}	3.62×10^{-6}	4.55×10^{-6}
Methenamine	100-97-0	−4.15	--	1.00×10^{6}	1.63×10^{-1}	--	1.64×10^{-9}
Methoxyacetic acid	625-45-6	−0.68	--	1.00×10^{6}	4.54×10^{-8}	8.68×10^{-9}	6.42×10^{-9}
Methyl salicylate	119-36-8	2.6	2.55	1,875	4.55×10^{-6}	2.23×10^{-9}	9.81×10^{-5}
Methyl vinyl ketone	78-94-4	0.41	--	6.06×10^{4}	2.61×10^{-5}	1.38×10^{-5}	4.65×10^{-5}
Methylcyclohexane	108-87-2	3.59	3.61	28.4	3.39×10^{-1}	3.30×10^{-1}	4.30×10^{-1}
Methylene bis(thiocyanate)	6317-18-6	0.62	--	2.72×10^{4}	2.61×10^{-8}	--	--
Methylenebis(5-methyloxazolidine)	66204-44-2	−0.58	--	1.00×10^{6}	1.07×10^{-7}	--	--
Morpholine	110-91-8	−0.56	−0.86	1.00×10^{6}	1.14×10^{-7}	3.22×10^{-9}	1.16×10^{-6}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	78-21-7	4.54	--	0.9381	2.66×10^{-12}	--	--
N-(2-Acryloyloxyethyl)-N-benzyl-N,N-dimethylammonium chloride	46830-22-2	−1.39	--	4.42×10^{5}	5.62×10^{-16}	--	--
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	−5.92	--	1.00×10^{6}	1.76×10^{-8}	--	--
N,N,N-Trimethyl-3-((1-oxooctadecyl)amino)-1-propanaminium methyl sulfate	19277-88-4	4.38	--	0.7028	2.28×10^{-16}	--	--
N,N,N-Trimethyloctadecan-1-aminium chloride	112-03-8	4.17	--	2.862	5.16×10^{-10}	--	--
N,N'-Dibutylthiourea	109-46-6	2.57	2.75	2,287	4.17×10^{-6}	--	--
N,N-Dimethyldecylamine oxide	2605-79-0	1.4	--	2,722	4.88×10^{-14}	--	--
N,N-Dimethylformamide	68-12-2	−0.93	−1.01	9.78×10^{5}	7.38×10^{-8}	--	7.39×10^{-8}
N,N-Dimethylmethanamine hydrochloride	593-81-7	0.04	0.16	1.00×10^{6}	3.65×10^{-5}	1.28×10^{-4}	1.04×10^{-4}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
N,N-Dimethyl-methanamine-N-oxide	1184-78-7	−3.02	--	1.00×10^{6}	3.81×10^{-15}	--	--
N,N-dimethyloctadecylamine hydrochloride	1613-17-8	8.39	--	0.008882	4.51×10^{-3}	3.88×10^{-2}	--
N,N'-Methylenebisacrylamide	110-26-9	−1.52	--	7.01×10^{4}	1.14×10^{-9}	--	--
Naphthalene	91-20-3	3.17	3.3	142.1	5.26×10^{-4}	3.70×10^{-4}	4.40×10^{-4}
Naphthalenesulfonic acid, bis(1-methylethyl)-	28757-00-8	2.92	--	43.36	9.29×10^{-10}	--	--
Naphthalenesulphonic acid, bis (1-methylethyl)-methyl derivatives	99811-86-6	4.02	--	3.45	1.13×10^{-9}	--	--
Naphthenic acid ethoxylate	68410-62-8	3.41	--	112.5	3.62×10^{-8}	2.74×10^{-9}	--
Nitrilotriacetamide	4862-18-4	−4.75	--	1.00×10^{6}	1.61×10^{-18}	--	--
Nitrilotriacetic acid	139-13-9	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	−3.81	--	7.39×10^{5}	1.19×10^{-16}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
N-Methyl-2-pyrrolidone	872-50-4	−0.11	−0.38	2.48×10^{5}	3.16×10^{-8}	--	3.20×10^{-9}
N-Methyldiethanolamine	105-59-9	−1.5	--	1.00×10^{6}	8.61×10^{-11}	2.45×10^{-14}	3.14×10^{-11}
N-Methylethanolamine	109-83-1	−1.15	−0.94	1.00×10^{6}	8.07×10^{-10}	2.50×10^{-10}	--
N-Methyl-N-hydroxyethyl-N-hydroxyethoxyethylamine	68213-98-9	−1.78	--	1.00×10^{6}	1.34×10^{-12}	5.23×10^{-17}	--
N-Oleyl diethanolamide	13127-82-7	6.63	--	0.1268	9.35×10^{-9}	1.94×10^{-12}	--
Oleic acid	112-80-1	7.73	7.64	0.01151	4.48×10^{-5}	1.94×10^{-5}	--
Pentaethylenehexamine	4067-16-7	−3.67	--	1.00×10^{6}	8.36×10^{-24}	2.56×10^{-27}	--
Pentane	109-66-0	2.8	3.39	49.76	1.29	1.20	1.25
Pentyl acetate	628-63-7	2.34	2.3	996.8	5.45×10^{-4}	4.45×10^{-4}	3.88×10^{-4}
Pentyl butyrate	540-18-1	3.32	--	101.9	9.60×10^{-4}	8.88×10^{-4}	--
Peracetic acid	79-21-0	−1.07	--	1.00×10^{6}	1.39×10^{-6}	--	2.14×10^{-6}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Phenanthrene	85-01-8	4.35	4.46	0.677	5.13×10^{-5}	2.56×10^{-5}	4.23×10^{-5}
Phenol	108-95-2	1.51	1.46	2.62×10^{4}	5.61×10^{-7}	6.58×10^{-7}	3.33×10^{-7}
Phosphonic acid (dimethylamino(methylene))	29712-30-9	−1.9	--	1.00×10^{6}	1.00×10^{-24}	--	--
Phosphonic acid, (((2-[(2-hydroxyethyl)(phosphonomethyl)amino)ethyl)imino]bis(methylene))bis-, compd. with 2-aminoethanol	129828-36-0	−6.73	--	1.00×10^{6}	5.29×10^{-42}	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, potassium salt	67953-76-8	−0.01	--	1.34×10^{5}	9.79×10^{-26}	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, tetrasodium salt	3794-83-0	−0.01	--	1.34×10^{5}	9.79×10^{-26}	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-	15827-60-8	−9.72	--	1.00×10^{6}	--	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-, ammonium salt (1:x)	70714-66-8	−9.72	--	1.00×10^6	--	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]tetrakis-, sodium salt	22042-96-2	−9.72	--	1.00×10^6	--	--	--
Phosphonic acid, [[(phosphonomethyl) imino]bis[6,1-hexanediylnitrilobis (methylene)]]tetrakis-	34690-00-1	−5.79	--	1.00×10^6	--	--	--
Phthalic anhydride	85-44-9	2.07	1.6	3,326	6.35×10^{-6}	--	1.63×10^{-8}
Poly(oxy-1,2-ethanediyl), .alpha.-(octylphenyl)-.omega.-hydroxy-, branched	68987-90-6	5.01	--	3.998	1.24×10^{-7}	1.07×10^{-6}	--
Potassium acetate	127-08-2	0.09	−0.17	4.76×10^5	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Potassium oleate	143-18-0	7.73	7.64	0.01151	4.48×10^{-5}	1.94×10^{-5}	--
Propane	74-98-6	1.81	2.36	368.9	7.30×10^{-1}	6.00×10^{-1}	7.07×10^{-1}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Propanol, 1(or 2)-(2-methoxymethylethoxy)-	34590-94-8	−0.27	--	4.27×10^{5}	1.15×10^{-9}	1.69×10^{-9}	--
Propargyl alcohol	107-19-7	−0.42	−0.38	9.36×10^{5}	5.88×10^{-7}	--	1.15×10^{-6}
Propylene carbonate	108-32-7	0.08	−0.41	2.58×10^{5}	3.63×10^{-4}	--	3.45×10^{-8}
Propylene pentamer	15220-87-8	6.28	--	0.05601	3.92×10^{-1}	1.09×10^{-3}	--
p-Xylene	106-42-3	3.09	3.15	228.6	6.56×10^{-3}	6.14×10^{-3}	6.90×10^{-3}
Pyrimidine	289-95-2	−0.06	−0.4	2.87×10^{5}	2.92×10^{-6}	--	--
Pyrrole	109-97-7	0.88	0.75	3.12×10^{4}	9.07×10^{-6}	7.73×10^{-6}	1.80×10^{-5}
Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides	68424-95-3	2.69	--	90.87	2.20×10^{-10}	--	--
Quinaldine	91-63-4	2.69	2.59	498.5	7.60×10^{-7}	2.13×10^{-6}	--
Quinoline	91-22-5	2.14	2.03	1,711	6.88×10^{-7}	1.54×10^{-6}	1.67×10^{-6}
Rhodamine B	81-88-9	6.03	--	0.0116	--	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium 1-octanesulfonate	5324-84-5	1.06	--	5,864	9.15×10^{-8}	--	--
Sodium 2-mercaptobenzothiolate	2492-26-4	2.86	2.42	543.4	3.63×10^{-8}	--	--
Sodium acetate	127-09-3	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Sodium benzoate	532-32-1	1.87	1.87	2,493	1.08×10^{-7}	4.55×10^{-8}	3.81×10^{-8}
Sodium bicarbonate	144-55-8	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium bis(tridecyl) sulfobutanedioate	2673-22-5	11.15	--	7.46×10^{-9}	8.51×10^{-11}	--	--
Sodium C14-16 alpha-olefin sulfonate	68439-57-6	4.36	--	2.651	4.95×10^{-7}	--	--
Sodium caprylamphopropionate	68610-44-6	−0.26	--	615.1	1.19×10^{-9}	2.45×10^{-10}	--
Sodium carbonate	497-19-8	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium chloroacetate	3926-62-3	0.34	0.22	1.95×10^{5}	1.93×10^{-7}	8.88×10^{-8}	9.26×10^{-9}
Sodium decyl sulfate	142-87-0	1.44	--	1,617	1.04×10^{-7}	--	--
Sodium D-gluconate	527-07-1	−1.87	--	1.00×10^{6}	4.74×10^{-13}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium diacetate	126-96-5	0.09	−0.17	4.76×10^{5}	5.48×10^{-7}	2.94×10^{-7}	1.00×10^{-7}
Sodium dichloroisocyanurate	2893-78-9	1.28	--	3,613	3.22×10^{-12}	--	--
Sodium dl-lactate	72-17-3	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Sodium dodecyl sulfate	151-21-3	2.42	--	163.7	1.84×10^{-7}	--	--
Sodium erythorbate (1:1)	6381-77-7	−1.88	−1.85	1.00×10^{6}	4.07×10^{-8}	--	--
Sodium ethasulfate	126-92-1	0.38	--	1.82×10^{4}	5.91×10^{-8}	--	--
Sodium formate	141-53-7	−0.46	−0.54	9.55×10^{5}	7.50×10^{-7}	5.11×10^{-7}	1.67×10^{-7}
Sodium hydroxymethanesulfonate	870-72-4	−3.85	--	1.00×10^{6}	4.60×10^{-13}	--	--
Sodium l-lactate	867-56-1	−0.65	−0.72	1.00×10^{6}	1.13×10^{-7}	--	8.13×10^{-8}
Sodium maleate (1:x)	18016-19-8	0.05	−0.48	1.04×10^{5}	1.35×10^{-12}	8.48×10^{-14}	--
Sodium N-methyl-N-oleoyltaurate	137-20-2	4.43	--	0.4748	1.00×10^{-12}	--	--
Sodium octyl sulfate	142-31-4	0.46	--	1.58×10^{4}	5.91×10^{-8}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium salicylate	54-21-7	2.24	2.26	3,808	1.42×10^{-8}	5.60×10^{-12}	7.34×10^{-9}
Sodium sesquicarbonate	533-96-0	−0.46	--	8.42×10^{5}	6.05×10^{-9}	--	--
Sodium thiocyanate	540-72-7	0.58	--	4.36×10^{4}	1.46×10^{-4}	--	--
Sodium trichloroacetate	650-51-1	1.44	1.33	1.20×10^{4}	2.39×10^{-8}	--	1.35×10^{-8}
Sodium xylenesulfonate	1300-72-7	−0.07	--	5.89×10^{4}	3.06×10^{-9}	--	--
Sorbic acid	110-44-1	1.62	1.33	1.94×10^{4}	5.72×10^{-7}	4.99×10^{-8}	--
Sorbitan sesquioleate	8007-43-0	14.32	--	2.31×10^{-11}	7.55×10^{-12}	1.25×10^{-16}	--
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	5.89	--	0.01914	1.42×10^{-12}	5.87×10^{-20}	--
Sorbitan, monooctadecanoate	1338-41-6	6.1	--	0.01218	1.61×10^{-12}	2.23×10^{-19}	--
Sorbitan, tri-(9Z)-9-octadecenoate	26266-58-0	22.56	--	1.12×10^{-19}	4.02×10^{-11}	2.68×10^{-13}	--
Styrene	100-42-5	2.89	2.95	343.7	2.76×10^{-3}	2.81×10^{-3}	2.75×10^{-3}
Sucrose	57-50-1	−4.27	−3.7	1.00×10^{6}	4.47×10^{-22}	--	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Sulfan blue	129-17-9	−1.34	--	50.67	1.31×10^{-26}	--	--
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	68955-19-1	3.9	--	5.165	4.29×10^{-7}	--	--
Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	68187-17-7	0.46	--	1.58×10^{4}	5.91×10^{-8}	--	--
Symclosene	87-90-1	0.94	--	4,610	6.19×10^{-11}	--	--
tert-Butyl hydroperoxide	75-91-2	0.94	--	1.97×10^{4}	1.60×10^{-5}	--	--
tert-Butyl perbenzoate	614-45-9	2.89	--	159.2	2.06×10^{-4}	--	--
Tetradecane	629-59-4	7.22	7.2	0.009192	1.65×10^{1}	2.68×10^{1}	9.20
Tetradecyldimethylbenzylammonium chloride	139-08-2	3.91	--	3.608	1.34×10^{-11}	--	--
Tetraethylene glycol	112-60-7	−2.02	--	1.00×10^{6}	4.91×10^{-13}	5.48×10^{-19}	--
Tetraethylenepentamine	112-57-2	−3.16	--	1.00×10^{6}	2.79×10^{-20}	4.15×10^{-23}	--

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	−5.03	--	1.00×10^{6}	9.17×10^{-13}	--	--
Tetramethylammonium chloride	75-57-0	−4.18	--	1.00×10^{6}	4.17×10^{-12}	--	--
Thiamine hydrochloride	67-03-8	0.95	--	3,018	8.24×10^{-17}	--	--
Thiocyanic acid, ammonium salt	1762-95-4	0.58	--	4.36×10^{4}	1.46×10^{-4}	--	--
Thioglycolic acid	68-11-1	0.03	0.09	2.56×10^{5}	1.94×10^{-8}	--	--
Thiourea	62-56-6	−1.31	−1.08	5.54×10^{5}	1.58×10^{-7}	--	1.98×10^{-9}
Toluene	108-88-3	2.54	2.73	573.1	5.95×10^{-3}	5.73×10^{-3}	6.64×10^{-3}
Tributyl phosphate	126-73-8	3.82	4	7.355	3.19×10^{-6}	--	1.41×10^{-6}
Tributyltetradecylphosphonium chloride	81741-28-8	11.22	--	7.90×10^{-7}	2.61×10^{-1}	--	--
Tridecane	629-50-5	6.73	--	0.02746	1.24×10^{1}	1.90×10^{1}	2.88
Triethanolamine	102-71-6	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Triethanolamine hydrochloride	637-39-8	−2.48	−1	1.00×10^{6}	4.18×10^{-12}	3.38×10^{-19}	7.05×10^{-13}
Triethanolamine hydroxyacetate	68299-02-5	−2.97	--	1.00×10^{6}	6.28×10^{-11}	--	--
Triethyl citrate	77-93-0	0.33	--	2.82×10^{4}	6.39×10^{-10}	--	3.84×10^{-9}
Triethyl phosphate	78-40-0	0.87	0.8	1.12×10^{4}	5.83×10^{-7}	--	3.60×10^{-8}
Triethylene glycol	112-27-6	−1.75	−1.75	1.00×10^{6}	3.16×10^{-11}	2.56×10^{-16}	--
Triethylenetetramine	112-24-3	−2.65	--	1.00×10^{6}	9.30×10^{-17}	6.74×10^{-19}	--
Triisopropanolamine	122-20-3	−1.22	--	1.00×10^{6}	9.77×10^{-12}	4.35×10^{-18}	--
Trimethanolamine	14002-32-5	−3.95	--	1.00×10^{6}	1.42×10^{-8}	--	--
Trimethylamine	75-50-3	0.04	0.16	1.00×10^{6}	3.65×10^{-5}	1.28×10^{-4}	1.04×10^{-4}
Tripotassium citrate monohydrate	6100-05-6	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Tripropylene glycol monomethyl ether	25498-49-1	−0.2	--	1.96×10^{5}	2.36×10^{-11}	4.55×10^{-13}	--
Trisodium citrate	68-04-2	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}

Chemical name	CASRN	Log K_{ow}		Water solubility	Henry's law constant (atm-m^3/mol at 25°C)		
		Estimated	Measured	Estimate from log K_{ow} (mg/L at 25°C)	Bond method	Group method 25	Measured
Trisodium citrate dihydrate	6132-04-3	−1.67	−1.64	1.00×10^{6}	8.33×10^{-18}	--	4.33×10^{-14}
Trisodium ethylenediaminetetraacetate	150-38-9	−3.86	--	2.28×10^{5}	1.17×10^{-23}	--	5.77×10^{-16}
Trisodium ethylenediaminetriacetate	19019-43-3	−4.32	--	1.00×10^{6}	3.58×10^{-20}	--	--
Tromethamine	77-86-1	−1.56	--	1.00×10^{6}	8.67×10^{-13}	--	--
Undecane	1120-21-4	5.74	--	0.2571	7.04	9.52	1.93
Urea	57-13-6	−1.56	−2.11	4.26×10^{5}	3.65×10^{-10}	--	1.74×10^{-12}
Xylenes	1330-20-7	3.09	3.2	207.2	6.56×10^{-3}	6.14×10^{-3}	7.18×10^{-3}

"--" indicates no information available.

The EPI (Estimation Programs Interface) Suite™ (U.S. EPA, 2012a) is an open-source, Windows®-based suite of physicochemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation. More information on EPI Suite™ is available at http://www.epa.gov/oppt/exposure/pubs/episuite.htm.

Although only physicochemical properties from EPI Suite™ are provided here, other sources of information were also consulted. QikProp (Schrodinger, 2012) and LeadScope® (Inc., 2012) are commercial products designed primarily as drug development and screening tools. QikProp is specifically focused on drug discovery and provides predictions for physically significant descriptors and pharmaceutically (and toxicologically) relevant properties useful in predicting ADME (adsorption, distribution, metabolism, and excretion) characteristics of drug candidates. QikProp's use of whole-molecule descriptors that have a straightforward physical interpretation (as opposed to fragment-based descriptors).

LeadScope® is a program designed for interpreting chemical and biological screening data that can assist pharmaceutical scientists in finding promising drug candidates. The software organizes the chemical data by structural features familiar to medicinal chemists. Graphs are used to summarize the data, and structural classes are highlighted that are statistically correlated with biological activity. It incorporates chemically-based data mining, visualization, and advanced informatics techniques (e.g., prediction tools, scaffold generators). Note that properties generated by QikProp and LeadScope® are generally more relevant to drug development than to environmental assessment.

Physicochemical properties of chemicals were generated from the two-dimensional (2-D) chemical structures from the EPA National Center for Computational Toxicology's Distributed Structure-Searchable Toxicity (NCCT DSSTox) Database Network in structure-data file (SDF) format. For EPI Suite™ properties, both the desalted and non-desalted 2-D files were run using the program's batch mode (i.e., processing many molecules at once) to calculate environmentally-relevant, chemical property descriptors. The chemical descriptors in QikProp require 3-D chemical structures. For these calculations, the 2-D desalted chemical structures were converted to 3-D using the Rebuild3D function in the Molecular Operating Environment software (CCG, 2011). All computed physicochemical properties are added into the structure-data file prior to assigning toxicological properties.

Both LeadScope® and Qikprop software require input of desalted structures. Therefore, the structures were desalted, a process where salts and complexes are simplified to the neutral, uncomplexed form of the chemical, using "Desalt Batch" option in ACD Labs ChemFolder. All LeadScope® general chemical descriptors (Parent Molecular Weight, AlogP, Hydrogen Bond Acceptors**,** Hydrogen Bond Donors, Lipinski Score, Molecular Weight, Parent Atom Count, Polar Surface Area, and Rotatable Bonds) were calculated by default.

All physicochemical properties generated from EPI Suite™, QikProp, and LeadScope® will be made available to the public in an electronic format in 2015.

C.2. References for Appendix C

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Appendix D

Designing, Constructing, and Testing Wells for Integrity

Appendix D. Designing, Constructing, and Testing Wells for Integrity

This appendix presents the goals for the design and construction of oil and gas production wells, the well components used to achieve those goals, and methods for testing well integrity to help verify that the goals for well performance are achieved. This information provides additional background for the well component discussions presented in Chapter 6. Information on the pathways associated with the well that can cause fluid movement into drinking water resources is presented in Chapter 6.

D.1. Design Goals for Well Construction

Simply stated, production wells are designed to move oil and gas from the production zone (within the oil and gas reservoir) into the well and then through the well to the surface. There are typically a variety of goals for well design (Renpu, 2011), but the main purposes are facilitating the flow of oil and gas from the hydrocarbon reservoirs to the well (production management) while isolating that oil and gas and the hydrocarbon reservoirs from nearby ground water resources (zonal isolation).

To achieve these goals, operators design and construct wells to have and maintain mechanical integrity throughout the life of the well. A properly designed and constructed well has two types of mechanical integrity: internal and external. Internal mechanical integrity refers to the absence of significant leakage within the production tubing, casing, or packer. External mechanical integrity refers to the absence of significant leakage along the well outside of the casing.

Achieving mechanical integrity involves designing the well components to resist the stresses they will encounter. Each well component must be designed to withstand all of the stresses to which the well will be subjected, including burst pressure, collapse, tensile, compression (or bending), and cyclical stresses (see Section 6.2.1 for additional information on these stresses). Well materials should also be compatible with the fluids (including liquids or gases) with which they come into contact to prevent leaks caused by corrosion.

These goals are accomplished by the use of one or more layers of casing, cement, and mechanical devices (such as packers), which provide the main barrier preventing migration of fluids from the well into drinking water sources.

D.2. Well Components

Casing and cement are used in the design and construction of wells to achieve the goals of mechanical integrity and zonal isolation. Several industry-developed specifications and best practices for well construction have been established to guide well operators in the construction process; see Text Box D-1. (Information is not available to determine how often these practices are used or how well they prevent the development of pathways for fluid movement to drinking water resources.) The sections below describe options available for casing, cement, and other well components.

Text Box D-1. Selected Industry-Developed Specifications and Recommended Practices for Well Construction in North America.

American Petroleum Institute (API)

- API Guidance Document HF1—Hydraulic Fracturing Operations—Well Construction and Integrity Guidelines (API, 2009a)
- API RP 10B-2—Recommended Practice for Testing Well Cements (API, 2013)
- API RP 10D-2—Recommended Practice for Centralizer Placement and Stop Collar Testing (API, 2004)
- API RP 5C1—Recommended Practices for Care and Use of Casing and Tubing (API, 1999)
- API RP 65-2—Isolating Potential Flow Zones during Well Construction (API, 2010a)
- API Specification 10A—Specification on Cements and Materials for Well Cementing (API, 2010b)
- API Specification 11D1—Packers and Bridge Plugs (API, 2009b)
- API Specification 5CT—Specification for Casing and Tubing (API, 2011)

Canadian Association of Petroleum Producers (CAPP) and Enform

- Hydraulic Fracturing Operating Practices: Wellbore Construction and Quality Assurance (CAPP, 2013)
- Interim Industry Recommended Practice Volume #24—Fracture Stimulation: Inter-wellbore Communication (Enform, 2013)

Marcellus Shale Coalition (MSC)

- Recommended Practices—Drilling and Completions (MSC, 2013)

D.2.1. Casing

Casing is steel pipe that is placed into the wellbore (the cylindrical hole drilled through the subsurface rock formation) to maintain the stability of the wellbore, to transport the hydrocarbons from the subsurface to the surface, and to prevent intrusion of other fluids into the well and wellbore. Up to four types of casing may be present in a well, including (from largest to smallest-diameter): conductor casing, surface casing, intermediate casing, and production casing. Each is described below.

The **conductor casing** is the largest diameter string of casing. It is typically in the range of 30 in. (76 cm) to 42 in. (107 cm) in diameter (Hyne, 2012). Its main purpose is to prevent unconsolidated material, such as sand, gravel, and soil, from collapsing into the wellbore. Therefore, the casing is typically installed from the surface to the top of the bedrock or other consolidated formations. The conductor casing may or may not be cemented in place.

The next string of casing is the **surface casing**. A typical surface casing diameter is 13.75 in. (34.93 cm), but diameter can vary (Hyne, 2012). The surface casing's main purposes are to isolate any ground water resources that are to be protected by preventing fluid migration along the wellbore

once the casing is cemented and to provide a sturdy structure to which blow-out prevention equipment can be attached. For these reasons, the surface casing most commonly extends from the surface to some distance beneath the lowermost geologic formation containing ground water resources to be protected. The specific depth to which the surface casing is set is often governed by the depth of the ground water resource as defined and identified for protection in state regulations.

Intermediate casing is typically used in wells to control pressure in an intermediate-depth formation. It may be used to reduce or prevent exposure of weak formations to pressure from the weight of the drilling fluid or cement or to allow better control of over-pressured formations. The intermediate casing extends from the surface through the formation of concern. There may be more than one string of concentric intermediate casing present or none at all, depending on the subsurface geology. Intermediate casing may be cemented, especially through over-pressured zones; however, it is not always cemented to the surface. Intermediate casing, when present, is often 8.625 in. (21.908 cm) in diameter but can vary (Hyne, 2012).

Production casing extends from the surface into the production zone. The main purposes of the production casing are to isolate the hydrocarbon product from fluids in surrounding formations and to transport the product to the surface. It can also be used to inject fracturing fluids, receive flowback during hydraulic fracturing operations (e.g., if tubing or a temporary fracturing string is not present), and prevent other fluids from mixing with and diluting the produced hydrocarbons. The production casing is generally cemented to some point above the production zone. Production casing is often 5.5 in. (14.0 cm) in diameter but can vary (Hyne, 2012).

Liners are another type of metal tubular (casing-like) well component that can be used to fulfill the same purposes as intermediate and production casing in the production zone. Like casing, they are steel pipe, but differ in that they do not extend from the production zone to the surface. Rather, they are connected to the next largest string of casing by a hanger that is attached to the casing. A frac sleeve is a specialized type of liner that is used during fracturing. It has plugs that can be opened and closed by dropping balls from the surface (see the discussion of well completions below for additional information on the use of frac sleeves).

Production tubing is the smallest, innermost steel pipe in the well and is distinguished from casing by not being cemented in place. It is used to transport the hydrocarbons to the surface. Fracturing may be done through the tubing if present, or through the production casing. Because casing cannot be replaced, tubing is often used, especially if the hydrocarbons contain corrosive substances such as hydrogen sulfide or carbon dioxide. Tubing may not be used in high-volume production wells. Typical tubing diameter is between 1.25 in. (3.18 cm) and 4.5 in. (11.4 cm) (Hyne, 2012).

D.2.2. Cement

Cement is the main barrier preventing fluid movement along the wellbore outside the casing. It also lends mechanical strength to the well and protects the casing from corrosion by naturally occurring formation fluids. Cement is placed in the annulus, which is the space between two adjacent casings or the space between the outermost casing and the rock formation through which the wellbore was

drilled. The sections below describe considerations for selecting cement and additives, as well as cementing procedures and techniques.

D.2.2.1. Considerations for Cementing

The length and location of the casing section to be cemented and the composition of the cement can vary based on numerous factors, including the presence and locations of weak formations, over- or under-pressured formations, or formations containing fluids; formation permeability; and temperature. State requirements for oil and gas production well construction and the relative costs of well construction options are also factors.

Improper cementing can lead to the formation of channels (small connected voids) in the cement, which can—if they extend across multiple formations or connect to other existing channels or fractures—present pathways for fluid migration. This section describes some of the considerations and concerns for proper cement placement and techniques and materials that are available to address these concerns. Careful selection of cements (and additives) and design of the cementing job can avoid integrity problems related to cement.

To select the appropriate cement type, properties, and additives, operators consider the required strength needed to withstand downhole conditions and compatibility with subsurface chemistry, as described below:

- The cement design needs to **achieve the strength** required under the measured or anticipated downhole conditions. Factors that are taken into account to achieve proper strength can include density, thickening time, the presence of free water, compressive strength, and formation permeability (Renpu, 2011). Commonly, cement properties are varied during the process, with a "weaker" (i.e., less dense) lead cement, followed by a "stronger" (denser) tail cement. The lead cement is designed with a lower density to reduce pressure on the formation and better displace drilling fluid without a large concern for strength. The stronger tail cement provides greater strength for the deeper portions of the well the operator considers as requiring greater strength.
- The **compatibility of the cement** with the chemistry of formation fluids, hydrocarbons, and hydraulic fracturing fluids is important for maintaining well integrity through the life of the well. Most oil and gas wells are constructed using some form of Portland cement. Portland cement is a specific type of cement consisting primarily of calcium silicates with additional iron and aluminum. Industry specifications for recommended cements are determined by the downhole pressure, temperature, and chemical compatibility required.

There are a number of considerations in the design and execution of a cement job. Proper centralization of the casing within the wellbore is one of the more important considerations. Others include the potential for lost cement, gas invasion, cement shrinkage, incomplete removal of drilling mud, settling of solids in the wellbore, and water loss into the formation while curing. These concerns, and techniques available to address them, include the following:

- **Improper centralization of the casing within the wellbore** can lead to preferential flow of cement on the side of the casing with the larger space and little to no cement on the side closest to the formation. If the casing is not centered in the wellbore, cement will flow unevenly during the cement job, leading to the formation of cement channels. Kirksey (2013) notes that, if the casing is off-center by just 25%, the cement job is almost always inadequate. Centralizers are used to keep the casing in the center of the hole and allow an even cement job. To ensure proper centralization, centralizers are placed at regular intervals along the casing (API, 2010a). Centralizer use is especially key in horizontal wells, as the casing will tend to settle (due to gravity) to the bottom of the wellbore if the casing is not centered (Sabins, 1990), leading to inadequate cement on the lower side.
- **Lost cement** (sometimes referred to as lost returns) refers to cement that moves out of the wellbore and into the formation instead of filling up the annulus between the casing and the formation. Lost cement can occur in weak formations that fail (fracture) under pressure of the cement or in particularly porous, permeable, or naturally fractured formations. Lost cement can result in lack of adequate cement across a water- or brine-bearing zone. To avoid inadequate placement of cement due to lost cement, records of nearby wells can be examined to determine zones where lost cement returns occur (API, 2009a). If records from nearby wells are not available, cores and logs may be used to identify any high-permeability or mechanically weak formations that might lead to lost cement. Steps can then be taken to eliminate or reduce loss of cement to the formation. Staged cementing (see below) can reduce the hydrostatic pressure on the formation and may avoid fracturing weak formations (Lyons and Pligsa, 2004). Additives are also available that will lessen the flow of cement into highly porous formations (API, 2010a; Ali et al., 2009).
- **Gas invasion and cement shrinkage** during cement setting can also cause channels and poor bonding. During the cementing process, the hydrostatic pressure from the cement column keeps formation gas from entering the cement. As the cement sets (hardens), the hydrostatic pressure decreases; if it becomes less than the formation pressure, gas can enter the cement, leading to channels. Cement also shrinks as it sets, which can lead to poor bonding and formation of microannuli. These problems can be avoided by using cement additives that increase setting time or expand to offset shrinkage (McDaniel et al., 2014; Wojtanowicz, 2008; Dusseault et al., 2000). Foamed cement can help alleviate problems with shrinkage, although care needs to be taken in cement design to ensure the proper balance of pressure between the cement column and formation (API, 2010a). Cement additives are also available that will expand upon contact with certain fluids such as hydrocarbons. These cements, termed self-healing cements, are relatively new but have shown early promise in some fields (Ali et al., 2009). Rotating the casing during cementing will also delay cement setting. Another technique called pulsation, where pressure pulses are applied to the cement while it is setting, also can delay cement setting and loss of hydrostatic pressure until the cement is strong enough to resist gas penetration (Stein et al., 2003).

- Another important issue is **removal of drilling mud**. If drilling mud is not completely removed, it can gather on one side of the wellbore and prevent that portion of the wellbore from being adequately cemented. The drilling mud can then be eroded away after the cement sets, leaving a channel. Drilling mud can be removed by circulating a denser fluid (spacer fluid) to flush the drilling mud out (Kirksey, 2013; Brufatto et al., 2003). Mechanical devices called scratchers can also be attached to the casing and the casing rotated or reciprocated to scrape drilling mud from the wellbore (Hyne, 2012; Crook, 2008). The spacer fluid, which is circulated prior to the cement to wash the drilling fluid out of the wellbore, must be designed with the appropriate properties and pumped in such a way that it displaces the drilling fluid without mixing with the cement (Kirksey, 2013; API, 2010a; Brufatto et al., 2003).
- Also of concern in horizontal wells is the possibility of **solids settling** at the bottom of the wellbore and free water collecting at the top of the wellbore. This can lead to channels and poor cement bonding. The cement slurry must be properly designed for horizontal wells to minimize free water and solids settling.
- If there is free water in the cement, pressure can cause **water loss into the formation,** leaving behind poor cement or channels (Jiang et al., 2012). In horizontal wells, free water can also accumulate at the top of the wellbore, forming a channel (Sabins, 1990). Minimizing free water in the cement design and using fluid loss control additives can help control loss of water (Ross and King, 2007).

D.2.2.2. Cement Placement Techniques

The primary cement job is most commonly conducted by pumping the cement down the inside of the casing, then out the bottom of the casing where it is then forced up the space between the outside of the casing and the formation. (The cement can also be placed in the space between two casings.) If **continuous cement** (i.e., a sheath of cement placed along the entire wellbore) is desired, cement is circulated through the annulus until cement that is pumped down the central casing flows out of the annulus at the surface. A spacer fluid is often pumped ahead of cement to remove any excess drilling fluid left in the wellbore; even if the operator does not plan to circulate cement to the surface, the spacer fluid will still return to the surface, as this is necessary to remove the drilling mud from the annulus. If neither the spacer fluid nor the cement returns to the surface, this indicates that fluids are being lost into the formation.

Staged cementing is a technique that reduces pressure on the formation by decreasing the height (and therefore the weight) of the cement column. This may be necessary if the estimated weight and pressure associated with standard cement emplacement could damage zones where the formation intersected is weak. The reduced hydrostatic pressure at the bottom of the cement column can also reduce the loss of water to permeable formations, improving the quality of the cement job. In multiple-stage cementing, cement is circulated to just below a cement collar placed between two sections of casing. A cement collar will have been placed between two sections of casing, just above, with ports that can be opened by dropping a weighted tool. Two plugs—which are often referred to as bombs or darts because of their shape—are then dropped. The first plug is

dropped, once the desired cement for the first stage has been pushed out of the casing by a spacer fluid. It closes the section of the well below the cement collar and stops cement from flowing into the lower portion of the well. The second plug (or opening bomb) opens the cement ports in the collar, allowing cement to flow into the annulus between the casing and formation. Cement is then circulated down the wellbore, out the cement ports, into the annulus, and up to the surface. Once cementing is complete, a third plug is dropped to close the cement ports, preventing the newly pumped cement from flowing back into the well (Lyons and Pligsa, 2004); see Figure D-1.

Another less commonly used primary cementing technique is **reverse circulation cementing.** This technique has been developed to decrease the force exerted on weak formations. In reverse circulation cementing, the cement is pumped down the annulus directly between the outside of the outermost casing and the formation. This essentially allows use of lower density cement and lower pumping pressures. With reverse circulation cementing, greater care must be taken in calculating the required cement, ensuring proper cement circulation, and locating the beginning and end of the cemented portion.

Another method used to cement specific portions of the well without circulating cement along the entire wellbore length is to use a **cement basket**. A cement basket is a device that attaches to the well casing. It is made of flexible material such as canvas or rubber that can conform to the shape of the wellbore. The cement basket acts as a one-way barrier to cement flow. Cement can be circulated up the wellbore past the cement basket, but when circulation stops the basket prevents the cement from falling back down the wellbore. Cement baskets can be used to isolate weak formations or formations with voids. They can also be placed above large voids such as mines or caverns with staged cementing used to cement the casing above the void.

If any deficiencies are identified, **remedial cementing** may be performed. The techniques available to address deficiencies in the primary cement job including cement squeezes or top-job cementing. A cement squeeze injects cement under high pressure to fill in voids or spaces in the primary cement job caused by high pressure, failed formations, or improper removal of drilling mud. Although cement squeezes can be used to fix deficiencies in the primary cement job, they require the well to be perforated, which can weaken the well and make it susceptible to degradation by pressure and temperature cycling as would occur during fracturing (Crescent, 2011). Another method of secondary cementing is the top job. In a top job, cement is pumped down the annulus directly to fill the remaining uncemented space when cement fails to circulate to the surface.

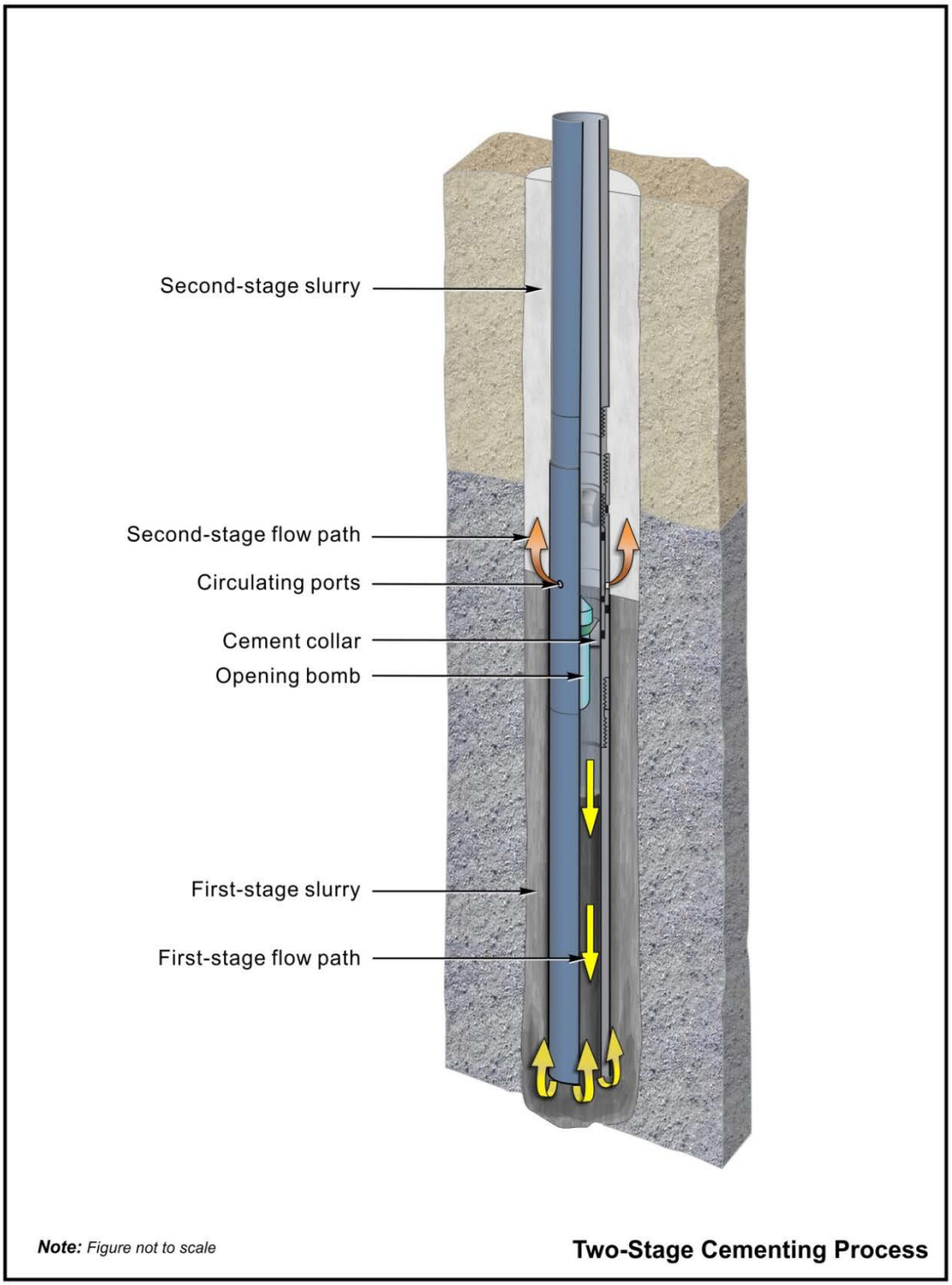

Figure D-1. A typical staged cementing process.

D.3. Well Completions

Completion refers to how the well is prepared for production and how flow is established between the formation and the surface. Figure D-2 presents examples of well completion types, including cased, formation packer, and open hole completion.

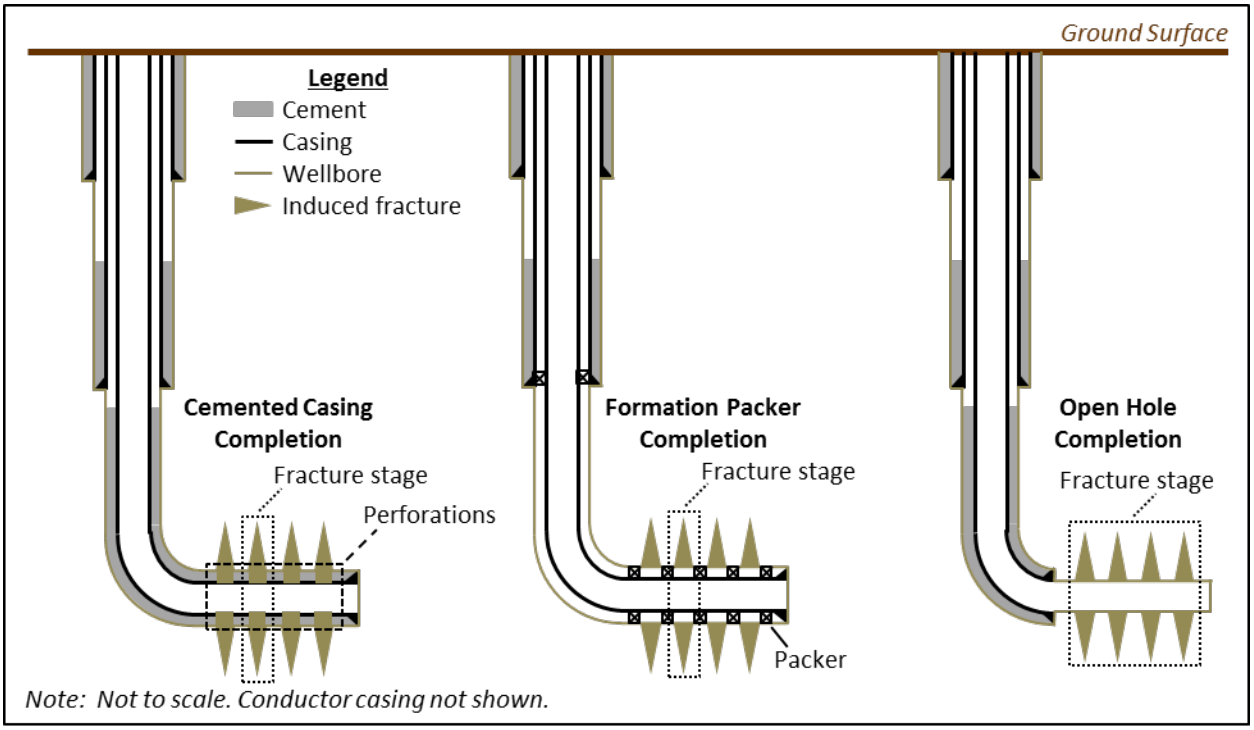

Figure D-2. Examples of well completion types.

Configurations shown include cased, formation packer, and open hole completion. From U.S. EPA (2015f).

A **cased completion**, where the casing extends to the end of the wellbore and is cemented in place, is the most common configuration of the well in the production zone (U.S. EPA, 2015f). Perforations are made through the casing and cement and into the formation using small explosive charges called "perf guns" or other devices, such as sand jets. Hydraulic fracturing then is conducted through the perforations. This is a common technique in wells that produce from several different depths and in low-permeability formations that are fractured (Renpu, 2011). While perforations do control the initiation point of the fracture, this can be a disadvantage if the perforations are not properly aligned with the local stress field. If the perforations are not aligned, the fractures will twist to align with the stress field, leading to tortuosity in the fractures and making fluid movement through them more difficult (Cramer, 2008). Fracturing stages can be isolated from each other using various mechanisms such as plugs or baffle rings, which close off a section of the well when a ball of the correct size is dropped down the well.

A packer is a mechanical device used to selectively seal off certain s ections of the wellbore. Packers can be used to seal the space between the tubing and casing, between two casings, or between the production casing and formation. The packer has one or more rubber elements that can be manipulated downhole to increase in diameter and make contact with the inner wall of the next-largest casing or the formation, effectively sealing the annulus created between the outside of the tubing and the inside of the casing. Packers vary in how they are constructed and how they are set, based on the downhole conditions in which they are used. There are two types of packers: internal packers and formation packers. Internal packers are used to seal the space between the casing and tubing or between two different casings. They isolate the outer casing layers from produced fluids and prevent fluid movement into the annulus. Formation packers seal the space between the casing and the formation and are often used to isolate fracture stages; they can be used to separate an open hole completion into separate fracture stages. Packers can seal an annulus by several different mechanisms. Mechanical packers expand mechanically against the formation and can exert a significant force on the formation. Swellable packers have elastomer sealing elements that swell when they come into contact with a triggering fluid such as water or hydrocarbons. They exert less force on the formation and can seal larger spaces but take some time to fully swell (McDaniel and Rispler, 2009). Internal mechanical integrity tests such as pressure tests can verify that the packer is functioning as designed and has not corroded or deteriorated.

In an **open hole completion**, the production casing extends just into the production zone and the entire length of the wellbore through the production zone is left uncased. This is only an option in formations where the wellbore is stable enough to not collapse into the wellbore. In formations that are unstable, a slotted liner may be used in open hole completions to control sand production (Renpu, 2011). Perforations are not needed in an open hole completion, since the production zone is not cased. An open hole completion can be fractured in a single stage or in multiple stages.

If formations are to be fractured in stages, additional completion methods are needed to separate the stages from each other and control the location of the fractures. One possibility is use of a liner with formation packers to isolate each stage. The liner is equipped with sliding sleeves that can be opened by dropping balls down the casing to open each stage. Fracturing typically occurs from the end of the well and continues toward the beginning of the production zone.

D.4. Mechanical Integrity Testing

While proper design and construction of the well's casing and cement are important, it is also important to verify the well was constructed and is performing as designed. Mechanical integrity tests (MITs) can verify that the well was constructed as planned and can detect damage to the production well that occurs during operations, including hydraulic fracturing activities. Verifying that a well has mechanical integrity can prevent potential impacts to drinking water resources by providing early warning of a problem with the well or cement and allowing repairs.

It is important to note that if a well fails an MIT, this does not mean the well has failed or that an impact on drinking water resources has occurred. An MIT failure is a warning that one or more components of the well are not performing as designed and is an indication that corrective actions

are necessary. If well remediation is not performed, a loss of well integrity could occur, which could result in fluid movement from the well.

D.4.1. Internal Mechanical Integrity

Internal mechanical integrity is an absence of significant leakage in the tubing, casing, or packers within the well system. Loss of internal mechanical integrity is usually due to corrosion or mechanical failure of the well's tubular and mechanical components.

Internal mechanical integrity can be tested by the use of pressure testing, annulus pressure monitoring, ultrasonic monitoring, and casing inspection logs or caliper logs:

- **Pressure testing** involves raising the pressure in the wellbore to a set level and shutting in the well. If the well has internal mechanical integrity, the pressure should remain constant with only small changes due to temperature fluctuation. Typically, the well is shut in (i.e., production is stopped and the wellhead valves closed) for half an hour, and if the pressure remains within 5% of the original reading, the well is considered to have passed the test. Usually, the well is pressure tested to the maximum expected pressure; for a well to be used for hydraulic fracturing this would be the pressure applied during hydraulic fracturing. Pressure tests, however, can cause debonding of the cement from the casing, so test length is often limited to reduce this effect (API, 2010a).
- If the annulus between the tubing and casing is sealed by a packer, **annulus pressure monitoring** can give an indication of the integrity of the tubing and casing. If the tubing, casing, and packer all have mechanical integrity, the pressure in the annulus should not change except for small changes in response to temperature fluctuations. The annulus can be filled with a non-corrosive liquid and the level of the liquid can be used as another indication of the integrity of the casing, tubing, and packer. The advantage of monitoring the tubing/production casing annulus is it can give a continuous, real-time indication of the internal integrity of the well. Even if the annulus is not filled with a fluid, monitoring its pressure can indicate leaks. If pressure builds up in the annulus and then recovers quickly after having bled off, that condition is referred to as sustained casing pressure or surface casing vent flow and is a sign of a leak in the tubing or casing (Watson and Bachu, 2009). Monitoring of annuli between other sets of casings can also provide information on the integrity of those casings. It can also provide information on external mechanical integrity for annuli open to the formation (see Section D.4.2 for additional information on external MITs). Jackson et al. (2013) also note that monitoring annular pressure allows the operator to vent gas before it accumulates enough pressure to cause migration into drinking water resources. Measuring annulus flow rate also allows detection of gas flowing into the annulus (Arthur, 2012).
- A newer tool uses **ultrasonic monitors** to detect leaks in casing and other equipment. It measures the attenuation of an ultrasonic signal as it is transmitted through the wellbore. The tool measures transmitted ultrasonic signals as it is lowered down the wellbore. The tool can pick up ultrasonic signals created by the leak, similar to noise logs. The tool only

has a range of a few feet but is claimed to detect leaks as small as half a cup per minute (Julian et al., 2007).

- **Caliper logs** have mechanical fingers that extend from a central tool and measure the distance from the center of the wellbore to the side of the casing. Running a caliper log can identify areas where corrosion has altered the diameter of the casing or where holes have formed in the casing. Caliper logs may also detect debris or obstructions in the well. Casing inspection and caliper logs are primarily used to determine the condition of the casing. Regular use of them may identify problems such as corrosion and allow mitigation before they cause of loss of integrity to the casing. To run these logs in a producing well, the tubing must first be pulled.
- **Casing inspection logs** are instruments lowered into the casing to inspect the casing for signs of wear or corrosion. One type of casing log uses video equipment to detect corrosion or holes. Another type uses electromagnetic pulses to detect variations in metal thickness. Running these logs in a producing well requires the tubing to be pulled.

If an internal mechanical integrity problem is detected, first, the location of the problem must be found. Caliper or casing inspection logs can detect locations of holes in casing. Locations of leaks can also be detected by sealing off different sections of the well using packers and performing pressure tests on each section until the faulty section is located. If the leaks are in the tubing or a packer, the problem may be remedied by replacing the well component. Casing leaks may be remedied by performing a cement squeeze (see the section on cementing).

D.4.2. External Mechanical Integrity

External well mechanical integrity is demonstrated by establishing the absence of significant fluid movement along the outside of the casing, either between the outer casing and cement or between the cement and the wellbore. Failure of an external MIT can indicate improper cementing or degradation of the cement emplaced in the annular space between the outside of the casing and the wellbore. This type of failure can lead to movement of fluids out of intended production zones and toward drinking water resources.

Several types of logs are available to evaluate external mechanical integrity, including temperature logs, noise logs, oxygen activation logs, radioactive tracer logs, and cement evaluation logs.

- **Temperature logs** measure the temperature in the wellbore. They are capable of measuring small changes in temperature. They can be performed using instruments that are lowered down the well on a wireline or they can be done using fiber optic sensors permanently installed in the well. When performed immediately after cementing, they can detect the heat from the cement setting and determine the location of the top of cement. After the cement has set, temperature logs can sense the difference in temperatures between formation fluids and injected or produced fluids. They may also detect temperature changes due to cooling or warming caused by flow. In this way temperature logs may detect movement of fluid outside the casing in the wellbore (Arthur, 2012).

Temperature logs require interpretation of the causes of temperature changes and are therefore subject to varying results among different users.

- **Noise logs** are sensitive microphones that are lowered down the well on a wireline. They are capable of detecting small noises caused by flowing fluids, such as fluids flowing through channels in the cement (Arthur, 2012). They are most effective at detecting fast-moving gas leaks and less successful with more slowly moving liquid migration.
- **Oxygen activation logs** consist of a neutron source and one or more detectors that are lowered on a wireline. The neutron source bombards oxygen molecules surrounding the wellbore and converts them into unstable nitrogen molecules that rapidly decay back to oxygen, emitting gamma radiation in the process. Gamma radiation detectors above or below the neutron source measure how quickly the oxygen molecules are moving away from the source, thereby determining flow associated with water.
- **Radioactive tracer logs** involve release of a radioactive tracer and then passing a detector up or down the wellbore to measure the path the tracers have taken. They can be used to determine if fluid is flowing up the wellbore. Tracer logs can be very sensitive but may be limited in the range over which leaks can be detected.
- **Cement evaluation logs** (also known as cement bond logs) are acoustic logs consisting of an instrument that sends out acoustic signals along with receivers, separated by some distance, that record the acoustic signals. As the acoustic signals pass through the casing they will be attenuated to an extent, depending on whether the pipe is free or is bonded to cement. By analyzing the return acoustic signal, the degree of cement bonding with the casing can be determined. The cement evaluation log measures the sound attenuation as sound waves passing through the cement and casing. There are different types of cement evaluation logs available. Some instruments can only return an average value over the entire wellbore. Other instruments are capable of measuring the cement bond radially. Cement logs do not actually determine whether fluid movement through the annulus is occurring. They only can determine whether cement is present in the annulus and in some cases can give a qualitative assessment of the quality of the cement in the annulus. Cement evaluation logs are used to calculate a bond index which varies between 0 and 1, with 1 representing the strongest bond and 0 representing the weakest bond.

If the well fails an external MIT, damaged or missing cement may be repaired using a cement squeeze (Wojtanowicz, 2008). A cement squeeze involves injection of cement slurry into voids behind the casing or into permeable formations. Different types of cement squeezes are available depending on the location of the void needing to be filled and well conditions (Kirksey, 2013). Cement squeezes are not always successful, however, and may need to be repeated to successfully seal off flow (Wojtanowicz, 2008).

D.5. References for Appendix D

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Appendix E

Flowback and Produced Water Supplemental Tables and Information

Appendix E. Flowback and Produced Water Supplemental Tables and Information

E.1. Flowback and Long-Term Produced Water Volumes

The EPA (2015g) estimates of flowback volumes and long-term produced water volumes used to generate the summaries appearing in Table 7-3 of Chapter 7 appear below in Table E-1.

Table E-1. Flowback and long-term produced water characteristics for wells in unconventional formations, formation-level data.

Source: U.S. EPA (2015g).

Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range[a]	Number of Data Points	Median	Range[b]	Number of Data Points
Anadarko	Shale	Woodford	H	4.7	1.0-12	2,239	34	20-50	3	5,500	3,200-6,400	198
	Tight	Cleveland	H	0.81	0.2-4.0	144	--	12-40	2	82	20-300	571
			V	0.69	0.11-3	4	--	--	2	32	6.6-170	390
		Granite Wash	H	6.2	0.2-9.4	77	--	7-22	2	1,300	0-2,200	273
			V	0.56	0.05-3	26	--	--	2	500	170-1,300	2,413
		Mississippi Lime	H	1.8	0.82-2.4	428	--	50	1	--	37,000-120,000	4
Appalachian	Shale	Marcellus	H	4.4	0.9-11	14,010	7	4-47	4,374	860	54-13,000	4,984
			V	2.6	0.53-6.6	66	40	21-60	7	230	100-1,200	714
		Utica	H	4.0	1.0-11	150	4	2-27	73	510	210-1,200	82
Arkoma	Shale	Fayetteville	H	5.1	1.7-11	1,668	--	10-20	2	430	150-2,300	2,305
Denver-Julesburg	Shale	Niobrara	H	2.6	0.73-3.4	69	13	6-25	16	680	260-810	250
			V	0.32	0.27-3.3	367	11	7-35	9	340	240-600	5,474
	Tight	Codell	D	0.28	0.21-0.46	78	--	--	0	--	--	0
			V	0.27	0.13-0.46	185	--	--	0	--	--	0
		Codell-Niobrara	H	2.6	0.15-2.7	62	7	--	32	34	19-140	32
			D	0.45	0.21-0.47	116	--	--	0	--	--	0
			V	0.30	0.13-0.46	592	--	--	0	29	13-65	1,677

Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range[a]	Number of Data Points	Median	Range[b]	Number of Data Points
Denver-Julesburg, cont.	Tight cont.	Muddy J	D	0.59	.025-0.62	162	--	--	0	230	64-390	3
			V	0.28	0.16-0.62	292	--	--	0	55	9.3-500	129
Fort Worth	Shale	Barnett	H	3.6	1-7.3	23,917	30	21-40	11	920	160-4,200	10,349
			V	1.3	0.4-1.9	3,589	--	--	0	250	170-580	3,318
Green River	Shale	Hilliard-Baxter-Mancos	H	1.7	1.0-5.6	2	--	--	0	37	15-58	7
	Tight	Lance	V	1.3	0.81-3.5	29	3	1-50	31	410	250-580	1,050
			D	1.2	0.76-1.9	180	6	1-17	170	860	360-1,200	1,140
Green River, cont.		Mesaverde	D	0.23	0.16-0.31	73	8	0-37	61	190	150-440	445
			V	0.17	0.081-0.29	14	21	6-83	11	290	140-610	1,081
Illinois	Shale	New Albany	H	--	--	0	--	--	0	--	2,900	2
Michigan	Shale	Antrim	V	--	0.05	1	--	25-75	2	--	4,600	1
Permian	Shale	Avalon & Bone Spring	D	2.2	0.94-4.5	20	13	5-31	16	950	220-2,400	183
			H	1.1	0.73-2.8	17	--	--	0	0	0-2,300	37
		Barnett-Woodford	H	2.1	0.5-4.5	2	--	--	0	--	--	0

Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range[a]	Number of Data Points	Median	Range[b]	Number of Data Points
Permian, cont.	Shale, cont.	Devonian (TX)	H	0.32	0.13-0.89	10	--	--	0	880	310-1,800	381
			V	0.27	0.12-1.0	16	--	--	0	400	150-3,000	162
		Wolfcamp	H	1.4	1.1-3.9	55	--	--	0	3,000	210-19,000	104
			D	1.3	0.26-1.7	12	16	15-20	3	310	22-8,700	259
			V	0.81	0.078-1.7	60	--	--	0	910	130-1,700	926
	Tight	Spraberry	V	--	1.0	1	--	--	0	870	100-4,000	66
San Juan	Tight	Mesaverde (San Juan)	D	--	--	0	--	--	0	18	12-260	48
		Dakota	V	0.2	0.063-0.22	19	--	--	0	65	29-120	6
			D	0.12	0.07-0.3	52	4	1-40	30	160	41-370	379
TX-LA-MS	Shale	Bossier	H	2.7	1.7-3.6	2	--	--	0	750	610-1,200	25
			V	0.4	0.19-1.7	16	--	--	0	470	180-1,100	1,203
			D	0.28	0.13-0.8	21	--	--	0	320	130-1,300	253
		Haynesville	H	5.3	0.95-15	3,222	5	5-30	3	1,700	84-1,800	1,249
			V	0.61	.14-3.5	9	--	--	0	210	56-850	263
	Tight	Cotton Valley	H	4.2	.25-6.0	30	--	<60	2	770	130-2,700	335
			D	.48	.084-4.0	24	--	<60	2	950	630-1,800	1801
			V	.28	.019-.94	76	--	<60	2	640	370-1,800	10,717

Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range[a]	Number of Data Points	Median	Range[b]	Number of Data Points
TX-LA-MS, cont.	Tight, cont.	Travis Peak	H	3.0	0.25-6	2	--	--	0	200	39-1,700	5
			V	0.9	0.2-4	2	--	--	0	980	330-1,800	1,380
Western Gulf	Shale	Eagle Ford	H	5.0	1.0-14	2,485	4	2-8	1,800	110	9.1-250	498
			V	2.9	2.0-4.1	9	--	--	0	--	--	0
		Pearsall	H	3.7	3.3-4.1	2	--	--	0	200	54-370	12
	Tight	Austin Chalk	H	0.94	0.58-1.3	15	--	--	0	720	290-2,400	1,097
		Vicksburg	V	.016	0.084-0.6	20	--	--	0	1,000	650-1,900	937
			D	0.11	0.1-0.13	4	--	--	0	--	--	0
		Wilcox Lobo	H	2.1	0.66-2.6	4	--	--	0	330	62-740	77
			V	0.21	0.06-0.6	14	--	--	0	620	330-1,400	1,514
			D	.058	.056-.076	3	--	--	0	--	--	0
		Olmos	V	--	0.15	2	--	--	0	--	--	0
Williston		Bakken	H	2.0	0.35-10	2,203	19	5-47	206	680	380-1,500	1,739
			V	1.1	.35-2.9	12	--	--	0	1,000	340-3,100	222

"--" indicates no data; H, horizontal well; D, directional well; V, vertical well.

[a] For some formations, if only one data point was reported, the EPA reported it in the range column and did not report a median value.

[b] For some formations, the number of data points was not reported in the data source. In these instances, the EPA reported the number of data points as equal to one, even if the source reported a range and median value.

E.2. Produced Water Content

E.2.1. Introduction

In the main text of Chapter 7, we describe aspects of flowback and produced water composition, including temporal changes in water quality parameters of flowback (Section 7.5) and major classes of compounds in produced water (Section 7.6). In section 7.7 we describe variability as occurring on three levels: between different rock types (e.g., coal vs. sandstone), between formations composed of the same rock types (e.g., Barnett Shale vs. Bakken Shale), and within formations of the same rock type (e.g., northeastern vs. southwestern Marcellus Shale). In this appendix we present data from the literature which illustrates the differences among these three variability levels.

E.2.2. General Water Quality Parameters

As noted in Chapter 7, the EPA identified data characterizing the content of unconventional flowback and produced water in a total of 12 shale and tight formations and coalbed methane (CBM) basins. These formations and basins span 18 states. Note that in this subsection we treat all fluids as produced water. As a consequence, the variability of reported concentrations is likely higher than if the data could be standardized to a specific point on the flowback-to-produced water continuum. Table E-2 and Table E-3 provide supporting data on general water quality parameters of produced water for 12 formations.

Table E-2. Reported concentrations of general water quality parameters in produced water for unconventional shale and tight formations, presented as: average (minimum–maximum) or *median* (minimum–maximum).

Parameter	Units	Shales					Tight formations			
		Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	**n/a**	**MT, ND**	**TX**	**AR**	**PA[d]**	**PA, WV[e]**	**LA, TX**	**PA**	**CO, NM, UT, WY**	**OK**
Acidity	mg/L	-	NC (ND–ND)	-	NC (<5–473)	***162*** (5–925)	-	-	-	-
Alkalinity	mg/L	-	***725*** (215–1,240)	1,347 (811–1,896)	165 (8–577)	***99.8*** (7.5–577)	-	99 (43–194)	-	582 (207–1,220)
Ammonium	mg/L	-	-	-	-	-	89 (40–131)	-	-	-
Bicarbonate	mg/L	291 (122–610)	-	-	-	-	-	524 (ND–8,440)	2,230 (1,281–13,650)	-
Biochemical oxygen demand (BOD)	mg/L	-	***582*** (101–2,120)	-	-	***141*** (2.8–12,400)	-	-	-	-
Carbonate	mg/L	-	-	-	-	-	-	-	227 (ND–1,680)	-
Chloride	mg/L	119,000 (90,000–133,000)	***34,700*** (9,600–60,800)	9,156 (5,507–12,287)	57,447 (64–196,000)	***49,000*** (64.2–196,000)	101,332 (3,167–221,498.7)	132,567 (58,900–207,000)	4,260 (8–75,000)	44,567 (23,000–75,000)
Chemical oxygen demand	mg/L	-	***2,945*** (927–3,150)	-	15,358 (195–36,600)	***4,670*** (195–36,600)	-	-	-	-

Parameter	Units	Shales					Tight formations			
		Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	**n/a**	**MT, ND**	**TX**	**AR**	**PA[d]**	**PA, WV[e]**	**LA, TX**	**PA**	**CO, NM, UT, WY**	**OK**
DO	mg/L	-	-	-	-	-	-	0.8 (0.2–2.5)	-	-
DOC	mg/L	-	***11.2*** (5.5–65.3)	-	-	***117*** (3.3–5,960)	-	-	-	-
Hardness as $CaCO_3$	mg/L	-	***5,800*** (3,500–21,000)	-	34,000 (630–95,000)	***25,000*** (156–106,000)	-	-	-	-
Oil and grease	mg/L	-	***163.5*** (88.2–1,430)	-	74 (5–802)	***16.85*** (4.7–802)	-	-	-	-
pH	SU	5.87 (5.47–6.53)	***7.05*** (6.5–7.2)	-	6.6 (5.1–8.4)	***6.5*** (4.9–7.9)	-	6.3 (5.5–6.8)	8 (5.8–11.62)	6.3 (6.1–6.4)
Specific conductivity	µS/cm	213,000 (205,000–220,800)	***111,500*** (34,800–179,000)	-	-	***183,000*** (479–763,000)	-	184,800 (118,000–211,000)	-	-
Specific gravity	--	1.13 (1.0961–1.155)	-	-	-	-	-	-	-	-
TDS	mg/L	196,000 (150,000–219,000)	***50,550*** (16,400–97,800)	13,290 (9,972–15,721)	106,390 (680–345,000)	***87,800*** (680–345,000)	164,683 (5,241–356,666)	235,125 (106,000–354,000)	15,802 (1,032–125,304)	73,082 (56,541–108,813)
Total Kjeldahl nitrogen	mg/L	-	***171*** (26–298)	-	-	***94.9*** (5.6–312)	-	-	-	-

Parameter	Units	Shales					Tight formations			
		Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	**n/a**	**MT, ND**	**TX**	**AR**	**PA[d]**	**PA, WV[e]**	**LA, TX**	**PA**	**CO, NM, UT, WY**	**OK**
TOC	mg/L	-	***9.75*** (6.2–36.2)	-	160 (1.2–1,530)	***89.2*** (1.2–5,680)	198 (184–212)	-	-	-
Total suspended solids	mg/L	-	***242*** (120–535)	-	352 (4–7,600)	***127*** (6.8–3,220)	-	-	-	-
Turbidity	NTU	-	***239*** (144–314)	-	-	***126*** (2.3–1,540)	-	-	-	-

n/a, not applicable; -, no value available; NC, not calculated; ND, not detected., SU= standard units, ***bolded italic*** numbers are medians

[a] Stepan et al. (2010). *n* = 3. Concentrations were calculated based on Stepan et al.'s raw data. Samples had charge balance errors of 1.74, -0.752, and -0.220%

[b] Hayes and Severin (2012b). *n* = 16. This data source reported concentrations without direct presentation of raw data.

[c] Warner et al. (2013). *n* = 6. Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

[d] Barbot et al. (2013). n = 134–159. This data source reported concentrations without direct presentation of raw data.

[e] Hayes (2009). *n* = 31-67. Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

[f] Blondes et al. (2014). Cotton Valley Group, *n*=2; Mesa Verde, *n* = 1–407; Oswego, *n* = 4–30. Concentrations were calculated based on raw data presented in the U.S. Geological Survey (USGS) National Produced Water Database v2.0.

[g] Dresel and Rose (2010). *n* = 3–15. Concentrations were calculated based on Dresel and Rose's raw data.

Table E-3. Reported concentrations of general water quality parameters in produced water for unconventional coalbed basins, presented as: average (minimum–maximum).

Parameter	Units	Black Warrior[a]	Powder River[b]	Raton[b]	San Juan[b]
States	n/a	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Alkalinity	mg/L	355 (3–1,600)	1,384 (653–2,672)	1,107 (130–2,160)	3,181 (51–11,400)
Ammonium	mg/L	3.60 (0.16–8.91)	-	-	-
Bicarbonate	mg/L	427 (2–1,922)	1,080 (236–3,080)	1,124 (127–2,640)	3,380 (117–13,900)
Carbonate	mg/L	3 (0–64)	2.17 (0.00–139.0)	51.30 (1.30–316.33)	40.17 (0.00–1,178)
Chloride	mg/L	9,078 (11–42,800)	21 (BDL–282)	787 (4.8–8,310)	624 (BDL–20,100)
Chemical oxygen demand	mg/L	830 (0–10,500)	-	-	-
Dissolved oxygen	mg/L	-	1.07 (0.11–3.48)	0.39 (0.01–3.52)	0.51 (0.04–1.69)
DOC	mg/L	3.37 (0.53–61.41)	3.18 (1.09–8.04)	1.26 (0.30–8.54)	3.21 (0.89–11.41)
Hardness as $CaCO_3$	mg/L	871 (3–6,150)	-	-	-
Hydrogen sulfide	mg/L	-	-	4.41 (BDL–190.0)	23.00 (23.00–23.00)
Oil and grease	mg/L	-	-	9.10 (0.60–17.6)	-
pH	SU	7.5 (5.3–9.0)	7.71 (6.86–9.16)	8.19 (6.90–9.31)	7.82 (5.40–9.26)
Phosphate	mg/L	0.435 (0.026–3.570)	BDL (BDL–BDL)	0.04 (BDL–1.00)	1.89 (BDL–9.42)
Specific conductivity	µS/cm	20,631 (718–97,700)	1,598 (413–4,420)	3,199 (742–11,550)	5,308 (232–18,066)
TDS	mg/L	14,319 (589–61,733)	997 (252–2,768)	2,512 (244–14,800)	4,693 (150–39,260)
Total Kjeldahl nitrogen	mg/L	6.08 (0.15–38.40)	0.48 (BDL–4.70)	2.61 (BDL–26.10)	0.46 (BDL–3.76)
TOC	mg/L	6.03 (0.00–103.00)	3.52 (2.07–6.57)	1.74 (0.25–13.00)	2.91 (0.95–9.36)
Total suspended solids	mg/L	78 (0–2,290)	11.0 (1.4–72.7)	32.3 (1.0–580.0)	47.2 (1.4–236.0)
Turbidity	NTU	74 (0–539)	8.2 (0.7–57.0)	4.5 (0.3–25.0)	61.6 (0.8–810.0)

n/a, not applicable; -, no value available; BDL, below detection limit.

[a] DOE (2014). *n* = 206. Concentrations were calculated based on raw data presented in the reference.

[b] Dahm et al. (2011). Powder River, *n* = 31; Raton, *n* = 40; San Juan, *n* = 20. This data source reported concentrations without presentation of raw data.

E.2.3. Salinity and Inorganics

Table E-4 and Table E-5 provide supporting data on salinity and inorganic constituents of produced water for 12 formations.

E.2.3.1. Processes Controlling Salinity and Inorganics Concentrations

Multiple mechanisms likely control elevated salt concentrations in flowback and produced water and are largely dependent upon post-injection fluid interactions and the formation's stratigraphic and hydrogeologic environment (Barbot et al., 2013). High inorganic ionic loads observed in flowback and produced water are expressed as TDS.

Subsurface brines or formation waters are saline fluids associated with the targeted formation. Shale and sandstone brines are typically much more saline than coalbed waters. After hydraulic fracturing fluids are injected into the subsurface, the injected fluids (which are typically not sources of high TDS) mix with in situ brines, which typically contain high ionic loads (Haluszczak et al., 2013).

Deep brines, present in over- or underlying strata, may naturally migrate into targeted formations over geologic time or artificially intrude if a saline aquifer is breached during hydraulic fracturing (Chapman et al., 2012; Maxwell, 2011; Blauch et al., 2009). Whether it is through natural or induced intrusion, saline fluids may contact the producing formation and introduce novel salinity sources to the produced water (Chapman et al., 2012).

The dissolution salts associated with formation solids both increases TDS concentrations and alters formation porosity and permeability (Blauch et al., 2009). Additionally, the mobilization of connate fluids (deposition-associated pore fluids) and formation fluids during hydraulic fracturing likely contributes to increased TDS levels (Dresel and Rose, 2010; Blauch et al., 2009). Despite the general use of fresh water for hydraulic fracturing fluid, some elevated salts in produced water may result from the use of reused saline flowback or produced water as a hydraulic fracturing base fluid (Hayes, 2009).

Table E-4. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in unconventional shale and tight formations produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).

Parameter	Shale					Tight Formations			
	Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	MT, ND	TX	AR	PA[d]	PA,WV[e]	LA, TX	PA	CO, NM, UT, WY	OK
Bromide	-	**589** (117–798)	111 (96–144)	511 (0.2–1,990)	***512*** (15.8–1,990)	498 (32–1,338)	1,048 (349–1,350)	-	-
Calcium	9,680 (7,540–13,500)	***1,600*** (1,110–6,730)	317 (221–386)	7,220 (38–41,000)	***7,465*** (173-33,000)	19,998 (181–51,400)	20,262 (8,930–34,400)	212 (1.01–4,580)	5,903 (3,609–8,662)
Chloride	119,000 (90,000–133,000)	***34,700*** (9,600–60,800)	9,156 (5,507–12,287)	57,447 (64–196,000)	***49,000*** (64.2–196,000)	101,332 (3,167–221,498.7)	132,567 (58,900–207,000)	4,260 (8–75,000)	44,567 (23,000–75,000)
Fluoride	-	***3.8*** (3.5–12.8)	-	-	***0.975*** (0.077–32.9)	-	-	-	-
Iodine	-	-	-	-	-	20 (1–36)	39 (11–56)	1.01 (1.01–1.01)	-
Nitrate as N	-	-	NC (ND–ND)	-	***1.7*** (0.65–15.9)	-	-	0.6 (0.6–0.6)	-
Nitrite as N	-	***4.7*** (3.5–38.1)	-	-	***11.8*** (1.1–146)	-	-	-	-
Phosphorus	NC (ND–0.03)	***0.395*** (0.19–0.7)	-	-	***0.3*** (0,08–21.8)	-	-	-	-
Potassium	2,970 (0–5,770)	***316*** (80–750)	-	-	***337*** (38–3,950)	1,975 (8–7,099)	858 (126–3,890)	160 (4–2,621)	-

Parameter	Shale					Tight Formations			
	Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	MT, ND	TX	AR	PA[d]	PA,WV[e]	LA, TX	PA	CO, NM, UT, WY	OK
Silica	7 (6.41–7)	-	52 (13–160)	-	-	4 (4–4)	-	-	-
Sodium	61,500 (47,100–74,600)	***18,850*** (4,370–28,200)	3,758 (3,152–4,607)	21,123 (69–117,000)	***21,650*** (63.8–95,500)	39,836 (1,320–85,623.24)	58,160 (24,400–83,300)	5,828 (132–48,817)	19,460 (13,484–31,328)
Sulfate	660 (300–1,000)	***709*** (120–1,260)	NC (ND–3)	71 (0–763)	***58.9*** (2.4–348)	407 (ND–2,200.46)	20 (1–140)	837 (ND–14,612)	183 (120–271)
Sulfide	-	NC (ND–ND)	-	-	***3.2*** (1.6–5.6)	-	0.7 (0.1–2.5)	-	-
Sulfite	-	-	-	-	***12.4*** (5.2–73.6)	-	-	-	-
TDS	196,000 (150,000–219,000)	*50,550* (16,400–97,800)	13,290 (9,972–15,721)	106,390 (680–345,000)	***87,800*** (680–345,000)	164,683 (5,241–356,666)	235,125 (106,000–354,000)	15,802 (1,032–125,304)	73,082 (56,541–108,813)

-, no value available; NC, not calculated; ND, not detected. ***Bolded italic*** numbers are medians.

[a] Stepan et al. (2010). *n* = 3. Concentrations were calculated based on Stepan et al.'s raw data. Samples had charge balance errors of 1.74, -0.752, and -0.220%

[b] Hayes and Severin (2012b). *n* = 16. This data source reported concentrations without presentation of raw data.

[c] Warner et al. (2013). *n* = 6. Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

[d] Barbot et al. (2013). *n* = 134–159. This data source reported concentrations without presentation of raw data.

[e] Hayes (2009). *n* = 8-65. Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

[f] Blondes et al. (2014) Cotton Valley Group, *n* = 2; Mesa Verde, *n* = 1–407; Oswego, *n* = 4–30. Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

[g] Dresel and Rose (2010). *n* = 3–15. Concentrations were calculated based on Dresel and Rose's raw data.

Table E-5. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in produced water for unconventional CBM basins, presented as: average (minimum–maximum).

Parameter	Black Warrior[a]	Powder River[b]	Raton[b]	San Juan[b]
State	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Barium	45.540 (0.136–352)	0.61 (0.14–2.47)	1.67 (BDL–27.40)	10.80 (BDL–74.0)
Boron	0.185 (0–0.541)	0.17 (BDL–0.39)	0.36 (BDL–4.70)	1.30 (0.21–3.45)
Bromide	-	0.09 (BDL–0.26)	4.86 (0.04–69.60)	9.77 (BDL–43.48)
Calcium	218 (0–1,640)	32.09 (2.00–154.0)	14.47 (0.81–269.0)	53.29 (1.00–5,530)
Chloride	9,078 (11–42,800)	21 (BDL–282)	787 (4.8–8,310)	624 (BDL–20,100)
Fluoride	6.13 (0.00–22.60)	1.57 (0.40–4.00)	4.27 (0.59–20.00)	1.76 (0.58–10.00)
Magnesium	68.12 (0.18–414.00)	14.66 (BDL–95.00)	3.31 (0.10–56.10)	15.45 (BDL–511.0)
Nitrate	8.70 (0.00–127.50)	-	-	-
Nitrite	0.03 (0.00–2.08)	-	-	-
Phosphorus	0.32 (0.00–5.76)	-	-	-
Potassium	12.02 (0.46–74.00)	11.95 (BDL–44.00)	6.37 (BDL–29.40)	26.99 (BDL–970.0)
Silica	8.66 (1.04–18.10)	6.46 (4.40–12.79)	7.05 (4.86–10.56)	12.37 (3.62–37.75)
Sodium	4,353 (126–16,700)	356 (12–1,170)	989 (95–5,260)	1,610 (36–7,834)
Strontium	11.354 (0.015–142.000)	0.60 (0.10–1.83)	5.87 (BDL–47.90)	5.36 (BDL–27.00)
Sulfate	5.83 (0.00–302.00)	5.64 (BDL–300.0)	14.75 (BDL–253.00)	25.73 (BDL–1,800)
TDS	14,319 (589–61,733)	997 (252–2,768)	2,512 (244–14,800)	4,693 (150–39,260)

-, no value available; BDL, below detection limit.

[a] DOE (2014). *n* = 206. Concentrations were calculated based on the authors' raw data.

[b] Dahm et al. (2011). Powder River, *n* = 31; Raton, *n* = 40; San Juan, *n* = 20. This data source reported concentrations without presentation of raw data.

E.2.4. Metals and Metalloids

Table E-6 and Table E-7 provide supporting data on metal constituents of produced water for 12 formations.

Table E-6. Reported concentrations (mg/L) of metals and metalloids from unconventional shale and tight formation produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).

Note that calcium, potassium, and sodium appear in Table E-4.

Parameter	Shale					Tight Formation			
	Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	MT, ND	TX	AR	PA[d]	PA, WV[e]	LA, TX	PA	CO, NM, UT, WY	OK
Aluminum	-	***0.43*** (0.37–2.21)	-	-	***2.5***7 (0.22–47.2)	-	-	-	-
Antimony	-	NC (ND–ND)	-	-	***0.028*** (0.018–0.038)	-	-	-	-
Arsenic	-	NC (ND–ND)	-	-	***0.101*** (0.013–0.124)	-	-	-	-
Barium	10 (0–24.6)	***3.6*** (0.93–17.9)	4 (3–5)	2,224 (0.24–13,800)	***542.5*** (2.590–13,900)	160 (ND–400.52)	1,488 (7–4,370)	139 (4–257)	
Beryllium	-	NC (ND–ND)	-	-	-	-	-	-	-
Boron	116 (39.9–192)	***30.3*** (7.0–31.9)	4.800 (2.395–21.102)	-	***12.2*** (0.808–145)	37 (2–100)	-	10 (1–14.2)	-
Cadmium	-	NC (ND–ND)	-	-	-	-	-	-	-
Chromium	-	***0.03*** (0.01–0.12)	-	-	***0.079*** (0.011–0.567)	-	-	-	-
Cobalt	-	***0.01*** (0.01–0.01)	-	-	-	-	-	-	-

Parameter	Shale					Tight Formation			
	Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	MT, ND	TX	AR	PA[d]	PA, WV[e]	LA, TX	PA	CO, NM, UT, WY	OK
Copper	NC (ND–0.21)	***0.29*** (0.06–0.52)	-	-	***0.506*** (0.253–4.150)	0.7 (0.48–1)	0.04 (0.01–0.13)	-	-
Iron	96 (ND–120)	***24.9*** (12.1–93.8)	7 (1–13)	-	***53.65*** (2.68–574)	-	188 (90–458)	9 (1–29)	61 (41–78)
Lead	-	***0.02*** (0.01–0.02)	-	-	***0.066*** (0.003–0.970)	-	0.02 (0.01–0.04)	-	-
Lithium	-	***19.0*** (2.56–37.4)	9.825 (2.777–28.145)	-	***53.85*** (3.410–323)	23 (1–53)	97.8 (20.2–315)	3 (1–33)	-
Magnesium	1,270 (630–1,750)	***255*** (149–755)	61 (47–75)	632 (17–2,550)	***678*** *(40.8–2,020)*	1,363 (27–3,712.98)	2,334 (797–3,140)	74 (1–2,394)	753 (486–1,264)
Manganese	7 (4–10.2)	***0.86*** (0.25–2.20)	2 (2–3)	-	***2.825*** (0.369–18.600)	30.33 (30.33–30.33)	19 (5.6–68)	-	-
Mercury	-	NC (ND–ND)	-	-	*0.00024*	-	-	-	-
Molybdenum	NC (ND–<0.2)	***0.02*** (0.02–0.03)	-	-	-	-	-	-	-
Nickel	-	***0.04*** (0.03–0.05)	-	***0.1815*** (0.007–0.137)	***0.419*** (0.068–0.769)	-	-	-	-
Selenium	-	***0.03*** (0.03–0.04)	-	-	*0.004*	-	-	-	-
Silver	-	-	-	-	***4*** *(3-6)*	-	-	-	-

Parameter	Shale					Tight Formation			
	Bakken[a]	Barnett[b]	Fayetteville[c]	Marcellus		Cotton Valley Group[f]	Devonian Sandstone[g]	Mesaverde[f]	Oswego[f]
States	MT, ND	TX	AR	PA[d]	PA, WV[e]	LA, TX	PA	CO, NM, UT, WY	OK
Strontium	764 (518–1,010)	***529*** (48–1,550)	27 (14–49)	1,695 (0.6–8,460)	***1,240*** (0.580–8,020)	2,312 (39–9,770)	3,890 (404–13,100)	-	-
Thallium	-	NC (ND–0.14)	-	-	*0.168*	-	-	-	-
Tin	-	NC (ND–ND)	-	-	-	-	-	-	-
Titanium	-	***0.02*** (0.02–0.03)	-	-	-	-	-	-	-
Zinc	7 (2–11.3)	***0.15*** (0.10–0.36)	-	-	***0.391*** (0.087–247)	-	0.20 (0.03–1.26)	-	-

-, no value available; NC, not calculated; ND, not detected; BDL, below detection limit. ***Bolded italic*** numbers are medians.

[a] Stepan et al. (2010). *n* = 3. Concentrations were calculated based on Stepan et al.'s raw data.

[b] Hayes and Severin (2012b). *n* = 16. This data source reported concentrations without presentation of raw data.

[c] Warner et al. (2013). *n* = 6. Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

[d] Barbot et al. (2013). *n* = 134–159. This data source reported concentrations without presentation of data.

[e] Hayes (2009). *n* = 48. Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

[f] Blondes et al. (2014). Cotton Valley Group, *n* = 2; Mesa Verde, *n* = 1–407; Oswego, *n* = 4–30. Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

[g] Dresel and Rose (2010). *n* = 3–15. Concentrations were calculated based on Dresel and Rose's raw data.

Table E-7. Reported concentrations (mg/L) of metals and metalloids from unconventional coalbed produced water, presented as: average (minimum–maximum).

Parameter	Black Warrior[a]	Powder River[b]	Raton[b]	San Juan[b]
States	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Aluminum	0.037 (0–0.099)	0.018 (BDL–0.124)	0.193 (BDL–2,900)	0.069 (BDL–0.546)
Antimony	0.006 (0.00–0.022)	BDL (BDL–BDL)	BDL (BDL–BDL)	BDL (BDL–BDL)
Arsenic	0.002 (0.0–0.085)	0.001 (BDL–0.004)	0.010 (BDL–0.060)	0.001 (BDL–0.020)
Barium	45.540 (0.136–352)	0.61 (0.14–2.47)	1.67 (BDL–27.40)	10.80 (BDL–74.0)
Beryllium	0.0 (0.0–0.008)	BDL (BDL–BDL)	BDL (BDL–BDL)	BDL (BDL–BDL)
Boron	0.185 (0–0.541)	0.17 (BDL–0.39)	0.36 (BDL–4.70)	1.30 (0.21–3.45)
Cadmium	0.001 (0.00–0.015)	BDL (BDL–0.002)	0.002 (BDL–0.003)	0.002 (BDL–.006)
Calcium	218 (0–1,640)	32.09 (2.00–154.0)	14.47 (0.81–269.0)	53.29 (1.00–5,530)
Cesium	0.011 (0.0–0.072)	-	-	-
Chromium	0.002 (0.0–0.351)	0.012 (BDL–0.250)	0.105 (BDL–3.710)	0.002 (BDL–0.023)
Cobalt	0.023 (0.00–0.162)	BDL (BDL–BDL)	0.001 (BDL–0.018)	0.001 (BDL–0.017)
Copper	0.001 (0.0–0.098)	0.078 (BDL–1.505)	0.091 (BDL–4.600)	0.058 (BDL–0.706)
Iron	8.956 (0.045–93.100)	1.55 (BDL–190.0)	7.18 (0.09–95.90)	6.20 (BDL–258.0)
Lead	0.008 (0.00–0.250)	BDL (BDL–BDL)	0.023 (BDL–0.233)	0.023 (BDL–0.390)
Lithium	1.157 (0–8.940)	0.13 (BDL–0.34)	0.32 (0.01–1.00)	1.61 (0.21–4.73)
Magnesium	68.12 (0.18–414.00)	14.66 (BDL–95.00)	3.31 (0.10–56.10)	15.45 (BDL–511.0)
Manganese	0.245 (0.006–4.840)	0.02 (BDL–0.16)	0.11 (0.01–2.00)	0.19 (BDL–1.34)
Mercury	0.000 (0.000–0.000)	-	-	-
Molybdenum	0.002 (0–0.083)	0.005 (BDL–0.029)	0.002 (BDL–0.035)	0.020 (BDL–0.040)
Nickel	0.015 (0.0–0.358)	0.141 (BDL–2.61)	0.015 (0.004–0.11)	0.020 (BDL–0.13)
Potassium	12.02 (0.46–74.00)	11.95 (BDL–44.00)	6.37 (BDL–29.40)	26.99 (BDL–970.0)
Rubidium	0.013 (0.0–0.114)	-	-	-
Selenium	0.002 (0.00–0.063)	0.006 (BDL–0.046)	0.017 (BDL–0.100)	0.018 (BDL–0.067)
Silver	0.015 (0.0–0.565)	0.003 (0.003–0.003)	0.015 (BDL–0.140)	BDL (BDL–BDL)
Sodium	4,353 (126–16,700)	356 (12–1,170)	989 (95–5,260)	1,610 (36–7,834)
Strontium	11.354 (0.015–142.000)	0.60 (0.10–1.83)	5.87 (BDL–47.90)	5.36 (BDL–27.00)
Thallium	-	-	-	-
Tin	0.00 (0.00–0.009)	0.006 (BDL–0.028)	0.008 (BDL–0.021)	0.017 (BDL–0.039)
Titanium	0.003 (0.0–0.045)	BDL (BDL–0.002)	BDL (BDL–0.002)	0.004 (BDL–0.020)

Parameter	Black Warrior[a]	Powder River[b]	Raton[b]	San Juan[b]
States	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Vanadium	0.001 (0.0–0.039)	BDL (BDL–BDL)	0.001 (BDL–0.013)	BDL (BDL–BDL)
Zinc	0.024 (0.0–0.278)	0.063 (BDL–0.390)	0.083 (0.010–3.900)	0.047 (0.005–0.263)

-, no value available; BDL, below detection limit.

[a] DOE (2014). *n* = 206. Concentrations were calculated based on the authors' raw data.

[b] Dahm et al. (2011). Powder River, *n* = 31; Raton, *n* = 40; San Juan, *n* = 20. This data source reported concentrations without presentation of raw data.

E.2.4.1. Processes Controlling Mineral Precipitation and Dissolution

Hydraulic fracturing treatments introduce fluids into the subsurface that are not in equilibrium with respect to formation mineralogy. Subsurface geochemical equilibrium modeling and saturation indices are therefore used to assess the solution chemistry of unconventional produced water and the subsequent likelihood of precipitation and dissolution reactions (Engle and Rowan, 2014; Barbot et al., 2013). Dissolution and precipitation reactions between fracturing fluids, formation solids, and formation water contribute to the chemistry of flowback and produced water.

For example, early flowback fluids may be under-saturated with respect to certain constituents or minerals associated with formation solids. Through time, as fluid-rock geochemistry returns to equilibrium, formation minerals will dissolve into solution and return in flowback.

Depending upon the formation chemistry and composition of the hydraulic fracturing fluid, the hydraulic fracturing fluid may initially have a lower ionic strength than existing formation fluids. Consequently, salts, carbonate, sulfate, and silicate minerals may undergo dissolution or precipitation. Proppants may also undergo dissolution or serve as nucleation sites for precipitation (McLin et al., 2011).

Currently, relatively little literature quantitatively explores subsurface dissolution and precipitation reactions between hydraulic fracturing fluids and formation solids and water. However, the processes that take place will likely be a function of the solubilities of the minerals, the chemistry of the fluid, pH, redox conditions, and temperature.

Documented dissolution processes in unconventional resources include the dissolution of feldspar followed by sodium enrichment in coalbed produced water (Rice et al., 2008). Dissolution of barium-rich minerals (barite ($BaSO_4$) and witherite ($BaCO_3$)), and strontium-rich minerals (celestite ($SrSO_4$) and strontianite ($SrCO_3$)) are known to enrich shale produced waters in barium and strontium (Chapman et al., 2012).

Known precipitation processes in unconventional resources include the precipitation of carbonate and subsequent reduction of calcium and magnesium concentrations in coalbed produced water (Rice et al., 2008). Additionally, calcium carbonate precipitation is suspected to cause declines in pH and alkalinity levels in shale produced water (Barbot et al., 2013).

The subsurface processes associated with fluid-rock interactions take place over a scale of weeks to months through the generation of flowback and produced water. Note that the types and extent of subsurface dissolution and precipitation reactions change with time, from injection through flowback and production. For instance, Engle and Rowan (2014) found that early Marcellus Shale flowback was under-saturated with respect to gypsum ($CaSO_4 \cdot 2H_2O$), halite (NaCl), celestite, strontianite, and witherite, indicating that these minerals would dissolve in the subsurface. Fluids were oversaturated with respect to barite. Saturation indices for gypsum, halite, celestite, and barite all increased during production. Knowing when dissolution and precipitation will likely occur is important, because dissolution and precipitation of minerals change formation permeability and porosity, which can affect production (André et al., 2006).

Additionally, pyrite (FeS_2) is an important minor mineral in reduced sedimentary rocks. Pyrite is the primary form of sulfur and iron occurrence in shales (Leventhal and Hosterman, 1982) and is also a common mineral phase generated in coals in which organic matter is closely associated (Ward, 2002). Pyrite content in shales can vary from less than 1% to several percent (Chermak and Schreiber, 2014; Vulgamore et al., 2007). Researchers have found a strong association of trace metals (i.e., nickel, copper, cadmium, chromium, cobalt, lead, selenium, vanadium, and zinc) with pyrite in shales (Chermak and Schreiber, 2014; Tuttle et al., 2009; Leventhal and Hosterman, 1982).

Although studies considering pyrite oxidation within the context of hydraulic fracturing are currently lacking, it is likely that the introduction of oxygenated fluids to freshly exposed surfaces in the subsurface during hydraulic fracturing can initiate limited, short-term pyrite oxidation or dissolution. Pyrite dissolution may increase iron and trace element concentrations and acidity in produced waters (Nordstrom and Alpers, 1999; Moses and Herman, 1991).

The extent to which the oxidative dissolution of pyrite would exert a control on post-injection subsurface fluid chemistry is unknown, although an ongoing U.S. Geological Survey (USGS) study anticipates it may be more significant than previously hypothesized (Li and Brantley, 2011). Regardless, relative to other reactions contributing to the composition of flowback and produced water (i.e., dissolution of salts), pyrite oxidation appears to be less significant. Ultimately, reactions resulting from temporary changes in subsurface redox conditions will be less important relative to other reactions that are less redox-dependent.

E.2.5. Naturally Occurring Radioactive Material (NORM) and Technically Enhanced Naturally Occurring Radioactive Material (TENORM)

E.2.5.1. Formation Solids Levels of NORM

Elevated uranium levels in formation solids have been used to identify potential areas of natural gas production for decades (Fertl and Chilingar, 1988). Marine black shales are estimated to contain an average of 5–20 ppm uranium depending on depositional conditions, compared to an average of less than 5 ppm among all shales (USGS, 1961). Shales that bear significant levels of uranium include the Barnett in Texas, the Woodford in Oklahoma, the New Albany in the Illinois Basin, the Chattanooga Shale in the southeastern United States, and a group of black shales in Kansas and Oklahoma (Swanson, 1955).

Bank et al. (2012) identified Marcellus samples with uranium ranging from 4–72 ppm, with an average of 30 ppm. Additionally, shale samples taken from three counties within the Marcellus Shale had uranium concentrations ranging from 8 to 84 ppm (BTGS, 2011; Hatch and Leventhal, 1981). Chermak and Schreiber (2014) compiled mineralogy and trace element data available in the literature for nine U.S. hydrocarbon-producing shales. In this combined data set, uranium levels among different shale plays were found to vary over three orders of magnitude, with samples of the Utica Shale containing approximately 0–5 ppm uranium and samples of the Woodford Shale containing uranium in the several-hundred-ppm range.

Vine (1956) reported that the principal uranium-bearing coal deposits of the United States are found in Cretaceous and Tertiary formations in the northern Great Plains and Rocky Mountains; in some areas of the West, coal deposits have been found with uranium concentrations in the range of thousands of ppm or greater. In contrast, most Mississippian, Pennsylvanian, and Permian coals in the north-central and eastern United States contain less than 10 ppm uranium, rarely containing 50 ppm or more.

E.2.5.2. Produced Water Levels of TENORM

Background data on NORM in the Marcellus Shale and Devonian sandstones are given in Table E-8.

Table E-8. Reported concentrations (in pCi/L) of radioactive constituents in unconventional shale and sandstone produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).

Parameter	Marcellus				Devonian Sandstone[a]
		PA NORM STUDY (PA DEP, 2015)			
States	NY, PA[b]	Flowback[c]	Conventional Produced Water[d]	Unconventional Produced Water[e]	PA
Gross alpha	***6,845*** (ND–123,000)	***10,700*** (288–71,000)	***1,835*** (465–2,570)	***11,300*** (2,240–41,700)	-
Gross beta	***1,170*** (ND–12,000)	***2,400*** (742–21,300)	***909*** (402–1,140)	***3.445*** (1.5–7,600)	-
Radium-226	***1,869*** (ND–16,920)	***4,500*** (551-25,500)	***243*** (81 – 819)	***6,300*** (1,700–26,600)	***2,367*** (200–5,000)
Radium-228	***557*** (ND–2,589)	***633*** (248–1,740)	***128*** (26 – 896)	***941*** (366–1,900)	-
Total Radium	***2,530*** (0.192-18,045)	-	***371*** (107 – 1,715)	***7,180*** (2,336–28,500)	-
Uranium^{235}	1 (ND–20)	-	-	-	-
Uranium^{238}	42 (ND–497)	-	-	-	-

n/a, not applicable; -, no value available; BDL, below detection limit. ***Bolded italic*** numbers are medians.

[a] Dresel and Rose (2010). *n* = 3. Concentrations presented were calculated based on Dresel and Rose's raw data.

[b] Rowan et al. (2011). *n* = 51. Concentrations presented were calculated based on Rowan et al.'s raw data for Marcellus samples. Uranium data from Barbot et al. (2013) *n* = 14.

[c] PA DEP (2015). n = 9. Data reported in Table 3-14.

[d] PA DEP (2015). n = 9. Values calculated from Table 3-15 for unfiltered samples.

[e] PA DEP (2015). n = 4. Values calculated from Table 3-15 for unfiltered samples.

E.2.5.3. Mobilization of Naturally Occurring Radioactive Material

Similar to conventional oil and gas production, in unconventional oil and gas production, radionuclides native to the targeted formation return to the surface with produced water. The principal radionuclides found in oil and gas produced waters include radium-226 of the uranium-238 decay series and radium-228 of the thorium-232 decay series (White, 1992). Levels of TENORM in produced water are controlled by geologic and geochemical interactions between injected and formation fluids, and the targeted formation (Bank, 2011). Mechanisms controlling NORM mobilization into produced water include (1) the TENORM content of the targeted formation; (2) factors governing the release of radionuclides, particularly radium, from the reservoir matrix; and (3) the geochemistry of the produced water (Choppin, 2007, 2006; Fisher, 1998).

Organic-rich shales and coals are enriched in uranium, thorium, and other trace metals in concentrations several times above those seen in typical shales or sedimentary rocks (Diehl et al., 2004; USGS, 1997; Wignall and Myers, 1988; Tourtelot, 1979; Vine and Tourtelot, 1970). Unlike shales and coals, sandstones are generally not organic-rich source rocks themselves. Instead, hydrocarbons migrate into these formations over long periods of time (Clark and Veil, 2009). Since TENORM and organic contents are typically positively correlated due to the original, reduced depositional environment (Fertl and Chilingar, 1988), it is unlikely that sandstones would be enriched in TENORM to the same extent as oil- and gas-bearing shales and coals. Therefore, concern related to TENORM within produced water is focused on operations targeting shales and coalbeds.

Radium is most soluble and mobile in chloride-rich, high-TDS, reducing environments (Sturchio et al., 2001; Zapecza and Szabo, 1988; Langmuir and Riese, 1985). In formation fluids with high TDS, calcium, potassium, magnesium, and sodium compete with dissolved radium for sorption sites, limiting radium sorption onto solids and allowing it to accumulate in solution at higher concentrations (Fisher, 1998; Webster et al., 1995). The positive correlation between TDS and radium is well established and TDS is a useful indicator of radium and TENORM activity within produced water, especially in lithologically homogenous reservoirs (Rowan et al., 2011; Sturchio et al., 2001; Fisher, 1998; Kraemer and Reid, 1984).

Uranium and thorium are poorly soluble under reducing conditions and are therefore more concentrated in formation solids than in solution (Fisher, 1998; Kraemer and Reid, 1984; Langmuir and Herman, 1980). However, because uranium becomes more soluble in oxidizing environments, the introduction of relatively oxygen-rich fracturing fluids may promote the temporary mobilization of uranium during hydraulic fracturing and early flowback. In addition, the physical act of hydraulic fracturing creates fresh fractures and exposes organic-rich and highly reduced surfaces from which radionuclides could be released from the rock into formation fluids.

Produced water geochemistry determines, in part, the fate of subsurface radionuclides, particularly radium. Radium may remain in the host mineral or it may be released into formation fluids, where it can remain in solution as the dissolved Ra^{2+} ion, be adsorbed onto oxide grain coatings or clay particles by ion exchange, substitute for other cations during the precipitation of minerals, or form

complexes with chloride, sulfate, and carbonate ions (Rowan et al., 2011; Sturchio et al., 2001; Langmuir and Riese, 1985). Uranium- and thorium-containing materials with a small grain size, a large surface-to-volume ratio, and the presence of uranium and thorium near grain surfaces promote the escape of radium into formation fluids. Vinson et al. (2009) point to alpha decay along fracture surfaces as a primary control on radium mobilization in crystalline bedrock aquifers. Radium may also occur in formation fluids due to other processes, such as the decay of dissolved parent isotopes and adsorption-desorption reactions on formation surfaces (Sturchio et al., 2001).

Preliminary results from fluid-rock interaction studies (Bank, 2011) indicate that a significant percentage of uranium in the Marcellus Shale may be subject to mobilization by hydrochloric acid, which is used as a fracturing fluid additive. Understanding these processes will determine the extent to which such processes might influence the TENORM content of flowback and produced water.

E.2.6. Organics

Background data on organics in seven formations is given in Table E-9.

Table E-9. Concentrations of select organic parameters from unconventional shale, a tight formation, and coalbed produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).

		Shale			Tight Formation	Coal			
Parameter	**Unit**	**Barnett[a]**	**Marcellus**		**Cotton Valley Group[d]**	**Powder River[e]**	**Raton[e]**	**San Juan[e]**	**Black Warrior[f]**
States	**n/a**	**TX**	**PA[b]**	**PA, WV[c]**	**LA, TX**	**MT, WY**	**CO, NM**	**AZ, CO, NM, UT**	**AL, MS**
TOC	mg/L	***9.75*** (6.2–36.2)	160 (1.2–1,530)	***89.2*** (1.2–5680)	198 (184–212)	3.52 (2.07–6.57)	1.74 (0.25–13.00)	2.91 (0.95–9.36)	6.03 (0.00–103.00)
DOC	mg/L	***11.2*** (5.5–65.3)	*43* (5–695)	***117*** (3.3–5,960)	-	3.18 (1.09–8.04)	1.26 (0.30–8.54)	3.21 (0.89–11.41)	3.37 (0.53–61.41)
BOD	mg/L	***582*** (101–2,120)	-	***141*** (2.8–12,400)	-	-	-	-	-
Oil and grease	mg/L	***163.5*** (88.2–1,430)	74 (5–802)	***16.9*** (4.7–802)	-	-	9.10 (0.60–17.6)	-	-
Benzene	µg/L	680 (49–5,300)	-	***220*** (5.8–2,000)	-	-	4.7 (BDL–220.0)	149.7 (BDL–500.0)	-
Toluene	µg/L	760 (79–8,100)	-	***540*** (5.1–6,200)	-	-	4.7 (BDL–78.0)	1.7 (BDL–6.2)	-
Ethylbenzene	µg/L	29 (2.2–670)	-	***42*** (7.6–650)	-	-	0.8 (BDL–18.0)	10.5 (BDL–24.0)	-

Parameter	Unit	Shale			Tight Formation	Coal			
		Barnett[a]	Marcellus		Cotton Valley Group[d]	Powder River[e]	Raton[e]	San Juan[e]	Black Warrior[f]
States	**n/a**	**TX**	**PA[b]**	**PA, WV[c]**	**LA, TX**	**MT, WY**	**CO, NM**	**AZ, CO, NM, UT**	**AL, MS**
Xylenes	µg/L	360 (43–1,400)	-	***300*** (15–6,500)	-	-	9.9 (BDL–190.0)	121.2 (BDL–327.0)	-
Average total BTEX[g]	µg/L	1,829	2,910	1,102	-	-	20.1	283.1	-

n/a, not applicable; -, no value available; BDL, below detection limit. ***Bolded italic*** numbers are medians.

[a] Hayes and Severin (2012b). *n* = 16. This data source reported concentrations without presentation of raw data.

b Barbot et al. (2013). *n* = 55; no presentation of raw data.

[c] Hayes (2009) *n* = 13-67. Concentrations were calculated based on Hayes' raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

[d] Blondes et al. (2014). *n* = 2. Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

[e] Dahm et al. (2011). Powder River, *n* = 31; Raton, *n* = 40; San Juan, *n* = 20. This data source reported concentrations without presentation of raw data.

[f] DOE (2014). n = 206. Concentrations were calculated based on the authors' raw data.

[g] Average total BTEX was calculated by summing the average/median concentrations of benzene, toluene, ethylbenzene, and xylenes for a unique formation or basin. Minimum to maximum ranges were not calculated due to inaccessible raw data.

Several classes of naturally occurring organic chemicals are present in conventional and unconventional produced waters, with large concentration ranges (Lee and Neff, 2011). These organic classes include total organic carbon (TOC); saturated hydrocarbons; BTEX (benzene, toluene, ethylbenzene, and xylenes); and polyaromatic hydrocarbons (PAHs) (see Table E-9). While TOC concentrations in produced water are detected at the milligrams to grams per liter level, concentrations of individual organic compounds are typically detected at the micrograms to milligrams per liter level.

TOC indicates the level of dissolved and undissolved organics in produced water, including non-volatile and volatile organics (Acharya et al., 2011). TOC concentrations in conventional produced water vary widely from less than 0.1 mg/L to more than 11,000 mg/L. Average TOC concentrations in unconventional produced water range from less than 2.00 mg/L in the Raton CBM basin to approximately 200 mg/L in the Cotton Valley Group sandstones, although individual measurements have exceeded 5,000 mg/L in the Marcellus Shale (see Table E-9).

Dissolved organic carbon (DOC) is a general indicator of organic loading and is the fraction of organic carbon available for complexing with metals and supporting microbial growth. DOC values in unconventional produced water range from less than 1.50 mg/L (average) in the Raton Basin to more than 115 mg/L (median) in the Marcellus Shale (see Table E-9). Individual DOC concentrations in the Marcellus Shale produced water approach 6,000 mg/L. For comparison, DOC levels in fresh water systems are typically below 5 mg/L, while raw wastewater can exceed 50 mg/L (Katsoyiannis and Samara, 2007; Muylaert et al., 2005).

Biochemical oxygen demand (BOD) is a conventional pollutant under the U.S. Clean Water Act. It is an indirect measure of biodegradable organics in produced water and an estimate of the oxygen demand on a receiving water. Median BOD levels for Barnett and Marcellus Shales produced water exceed 30 mg/L, and both reported maximum concentrations exceeding 12,000 mg/L (Table E-9). In some circumstances wide variation in produced water median BOD levels may be reflective of flowback reuse in fracturing fluids (Hayes, 2009).

Lastly, BTEX is associated with petroleum. Benzene was found in produced water from several basins: average produced water benzene concentration from the Barnett Shale was 680 μg/L, from the Marcellus Shale was 220 μg/L (median), and from the San Juan Basin was 150 μg/L (see Table E-9). Total BTEX concentrations for conventional produced water vary widely from less than 100 μg/L to nearly 580,000 μg/L. For comparison, average total BTEX concentrations in unconventional produced water range from 20 μg/L in the Raton Basin to nearly 3,000 μg/L in the Marcellus play (see Table E-9). From these data, average total BTEX levels in shale produced water are one to two orders of magnitude higher than those in CBM produced water.

In addition to abundant BTEX, a variety of volatile and semi-volatile organic compounds VOCs and SVOCs have been detected in shale and coalbed produced water. Shale produced water contains naphthalene, alkylated toluenes, and methylated aromatics in the form of several benzene and phenol compounds, as shown in Table E-10. Like BTEX, naphthalene, methylated phenols, and acetophenone are associated with petroleum. Detected shale produced water organics such as

acetone, 2-butanone, carbon disulfide, and pyridine are potential remnants of chemical additives used as friction reducers or industrial solvents (Hayes, 2009).

Table E-10. Reported concentrations (µg/L) of organic constituents in produced water for two unconventional shale formations, presented as: average (minimum–maximum) or *median* (minimum–maximum).

Parameter	Barnett[a]	Marcellus[b]
States	TX	MD, NY, OH, PA, VA, WY
Acetone	145 (27–540)	***83*** (14–5,800)
Carbon disulfide	-	***400*** (19–7,300)
Chloroform	-	28
Isopropylbenzene	35 (0.8–69)	***120*** (86–160)
Naphthalene	238 (4.8–3,100)	***195*** (14–1,400)
Phenolic compounds	***119.65*** (9.3–230)	-
1,2,4-Trimethylbenzene	173 (6.9–1,200)	***66.5*** (7.7–4,000)
1,3,5-Trimethylbenzene	59 (6.4–300)	***33*** (5.2–1,900)
1,2-Diphenylhydrazine	4.2 (0.5–7.8)	-
1,4-Dioxane	6.5 (3.1–12)	-
2-Methylnaphthalene	1,362 (5.4–20,000)	***3.4*** (2–120)
2-Methylphenol	28.3 (5.8–76)	***13*** (11–15)
2,4-Dichlorophenol	(ND–15)	-
2,4-Dimethylphenol	14.5 (8.3–21)	12
3-Methylphenol and 4-Methylphenol	41 (7.8–100)	***11.5*** (0.35-16)
Acetophenone	(ND–4.6)	***13*** (10–22)
Benzidine	(ND–35)	-
Benzo(a)anthracene	(ND–17.0)	-
Benzo(a)pyrene	(ND–130.0)	6.7
Benzo(b)fluoranthene	42.2 (0.5–84.0)	10
Benzo(g,h,i)perylene	42.3 (0.7–84.0)	6.9
Benzo(k)fluoranthene	32.8 (0.6–65.0)	5.9
Benzyl alcohol	81.5 (14.0–200)	***41*** (17–750)
Bis(2-Ethylhexyl) phthalate	210 (4.8–490)	***20*** (9.6–870)
Butyl benzyl phthalate	34.3 (1.9–110)	-

Parameter	Barnett[a]	Marcellus[b]
States	TX	MD, NY, OH, PA, VA, WY
Chrysene	120 (0.57–240)	-
Di-n-octyl phthalate	(ND–270)	15
Di-n-butyl phthalate	41 (1.5–120)	***14*** (11–130)
Dibenz(a,h)anthracene	77 (3.2–150)	***3.2*** (2.3–11)
Diphenylamine	5.3 (0.6–10.0)	-
Fluoranthene	(ND–0.18)	6.1
Fluorene	0.8 (0.46–1.3)	8.4
Indeno(1,2,3-cd)pyrene	71 (2.9–140)	***3.1*** (2.4–9.5)
N-Nitrosodiphenylamine	8.9 (7.8–10)	2.7
N-Nitrosomethylethylamine	(ND–410)	-
Phenanthrene	107 (0.52–1,400)	***9.75*** (3–22)
Phenol	63 (17–93)	***10*** (2.4–21)
Pyrene	0.2 (ND–0.18)	13
Pyridine	413 (100–670)	***250*** (10–2,600)

-, no value available; ND, not detected.

[a] Hayes and Severin (2012b). *n* = 16. Data from days 1–23 of flowback. This data source reported concentrations without presentation of raw data.

[b] Hayes (2009). *n* = 1-35. Data from days 1–90 of flowback. Concentrations were calculated from Hayes' raw data. Non-detects and contaminated blanks omitted.

The organic profile of CBM produced water is characterized by high levels of aromatic and halogenated compounds compared to other unconventional produced waters (Sirivedhin and Dallbauman, 2004). PAHs and phenols are the most common organic compounds found in coalbed produced water. Produced water from coalbeds in the Black Warrior Basin mainly contains phenols, multiple naphthalic PAHs, and various decanoic and decenoic fatty acids (see Table E-11). CBM-associated organics are also known to include biphenyls, alkyl aromatics, hydroxypyridines, aromatic amines, and nitrogen-, oxygen-, and sulfur-bearing heterocyclics (Orem et al., 2014; Pashin et al., 2014; Benko and Drewes, 2008; Orem et al., 2007; Fisher and Santamaria, 2002).

Table E-11. Reported concentrations of organic constituents in 65 samples of produced water from the Black Warrior CBM Basin, presented as average (minimum–maximum).

Parameter	Number of observations	Concentration (μg/L)[a]
States	-	AL, MS
Benzothiazole	45	0.25 (0.01–3.04)
Caprolactam	10	0.75 (0.02–2.39)
Cyclic octaatomic sulfur	29	1.06 (0.10–9.63)
Dimethyl-naphthalene	39	0.79 (0.01–9.51)
Dioctyl phthalate	57	0.21 (0.01–2.30)
Dodecanoic acid	30	1.13 (0.67–2.52)
Hexadecanoic acid	50	1.58 (1.17–3.02)
Hexadecenoic acid	25	1.69 (1.13–8.37)
Methyl-biphenyl	18	0.25 (0.01–2.13)
Methyl-naphthalene	52	0.77 (0.01–15.55)
Methyl-quinoline	31	0.96 (0.03–3.75)
Naphthalene	49	0.41 (0.01–6.57)
Octadecanoic acid	32	1.95 (1.62–3.73)
Octadecenoic acid	29	1.87 (1.60–3.47)
Phenol, 2,4-bis(1,1-dimethyl)	21	0.45 (0.01–4.94)
Phenol, 4-(1,1,3,3-tetramethyl)	17	1.65 (0.01–18.34)
Phenolic compounds	-	19.06 (ND–192.00)
Tetradecanoic acid	53	1.51 (0.94–5.32)
Tributyl phosphate	23	0.26 (0.01–2.66)
Trimethyl-naphthalene	23	0.65 (0.01–4.49)
Triphenyl phosphate	6	1.18 (0.01–6.77)

-, no value available.

[a] DOE (2014). Concentrations were calculated based on the authors' raw data.

Hayes (2009) characterized the content of Marcellus Shale produced water including organics (see Table E-10). The author tested for the majority of VOCs and SVOCs, pesticides and PCBs, based on the recommendation of the Pennsylvania and West Virginia Departments of Environmental Protection. Only 0.5% of VOCs and 0.03% of SVOCs in the produced water were detected above 1 mg/L. Approximately 96% of VOCs, 98% of SVOCs, and virtually all pesticides and PCBs were at nondetectable levels.

E.2.7. Chemical Reactions

Section E.2.7.1 describes general aspects of subsurface chemical reactions that might occur during hydraulic fracturing operations. Here we augment the discussion by describing subsurface chemical processes.

E.2.7.1. Injected Chemical Processes

Hydraulic fracturing injects relatively oxygenated fluids into a reducing environment, which may mobilize trace or major constituents into solution. Injection of oxygenated fluids may lead to short-term changes in the subsurface redox state, as conditions may shift from reducing to oxidizing. The chemical environment in hydrocarbon-rich unconventional reservoirs, such as black shales, is generally reducing, as evidenced by the presence of pyrite and methane (Engle and Rowan, 2014; Dresel and Rose, 2010). For black shales, reducing conditions are a product of original accumulations of organic matter whose decay depleted oxygen to create rich organic sediments within oil- and gas-producing formations (Tourtelot, 1979; Vine and Tourtelot, 1970). Yet reactions resulting from temporary redox shifts are likely to be less important than those resulting from other longer-term physical and geochemical processes. Temporary subsurface redox shifts may be due to the short timeframe for fluid injection (a few days to a few weeks) and the use of oxygen scavengers to prevent downhole equipment corrosion.

Hydraulic fracturing fluid injection introduces novel chemicals into the subsurface.[1] As such, the geochemistry of injected and native fluids will not be in equilibrium. Over the course of days to months, a complex series of reactions will equilibrate disparate fluid chemistries. The evolution of flowback and produced water geochemistry are dependent upon the exposure of formation solids and fluids to novel chemicals within hydraulic fracturing fluid. Chemical additives interact with reservoir solids and either mobilize constituents or themselves become adsorbed to solids. Such additives include metallic salts, elemental complexes, salts of organic acids, organometallics, and other metal compounds (Montgomery, 2013; House of Representatives, 2011).

The salts, elemental complexes, organic acids, organometallics, and other metal-containing compounds may interact with metals and metalloids in the target formation through processes such as ion exchange, adsorption, desorption, chelation, and complexation. For instance, natural organic ligands (e.g., citrate) are molecules that can form coordination compounds with heavy metals such as cadmium, copper, and lead (Martinez and McBride, 2001; Stumm and Morgan, 1981; Bloomfield et al., 1976). Citrate-bearing compounds are used in hydraulic fracturing fluids as surfactants, iron control agents, and biocides. Studies of the additives' interactions with formation solids at concentrations representative of hydraulic fracturing fluids are lacking.

Furthermore, pH will likely play a role in the nature and extent of these processes, as the low pH of hydraulic fracturing fluids may mobilize trace constituents. The pH of injected fluids may differ from existing subsurface conditions due to the use of dilute acids (e.g., hydrochloric or acetic) used for cleaning perforations and fractures during hydraulic fracturing treatments (Montgomery, 2013;

[1] For more information on chemical additive usage, refer to Chapter 5 (Chemical Mixing).

GWPC and ALL Consulting, 2009). Metals within formation solids may be released through the dissolution of acid-soluble phases such as iron and manganese oxides or hydroxides (Yang et al., 2009; Kashem et al., 2007; Filgueiras et al., 2002). Thus, the pH of hydraulic fracturing fluids, or changes in system pH that may occur as fluid recovery begins, may influence which metals and metalloids are likely to be retained within the formation and which may be recovered in flowback. Ultimately, more research is needed to fully understand how the injection of hydraulic fracturing fluids affects subsurface geochemistry and resultant flowback and produced water chemistry.

E.2.8. Microbial Community Processes and Content

By design, hydraulic fracturing releases hydrocarbons and other reduced mineral species from freshly fractured shale, sandstone, and coal, resulting in saltier in situ fluids, the release of formation solids, and increased interconnected fracture networks with rich colonization surfaces that are ideal for microbial growth (Wuchter et al., 2013; Curtis, 2002). Depending upon the formation, microorganisms may be native to the subsurface and/or introduced from non-sterile equipment and fracturing fluids. Additionally, microorganisms compete for novel organics in the form of chemical additives (Wuchter et al., 2013; Arthur et al., 2009). Since large portions of hydraulic fracturing fluid can remain emplaced in the targeted formation, long-term microbial activity is supported through these novel carbon and energy resources (Orem et al., 2014; Murali Mohan et al., 2013a; Struchtemeyer and Elshahed, 2012; Bottero et al., 2010). Such physical and chemical changes to the environment at depth stimulate microbial activity and influence flowback and produced water content in important ways.

Several studies characterizing produced water from unconventional formations (i.e., the Barnett, Marcellus, Utica, and Antrim Shales) indicate that taxa with recurring physiologies compose shale flowback and produced water microbial communities (Murali Mohan et al., 2013b; Wuchter et al., 2013). Such physiologies include sulfur cyclers (e.g., sulfidogens: sulfur , sulfate , and thiosulfate reducers); fermenters; acetogens; hydrocarbon oxidizers; methanogens; and iron, manganese, and nitrate reducers (Davis et al., 2012).

Based on their physiologies, microorganisms cycle substrates at depth by mobilizing or sequestering constituents in and out of solution. Mobilization can occur through biomethylation, complexation, and leaching. Sequestration can occur through intracellular sequestration, precipitation, and sorption to biomass.

The extent to which constituents are mobilized or sequestered depends upon the prevailing geochemical environment after hydraulic fracturing and through production. Significant environmental factors that influence the extent of microbially mediated reactions are increases in ionic content (i.e., salinity, conductivity, total nitrogen, bromide, iron, and potassium); decreases in acidity, and organic and inorganic carbon; the availability of diverse electron acceptors and donors; and the availability of sulfur-containing compounds (Cluff et al., 2014; Murali Mohan et al., 2013b; Davis et al., 2012). Examples follow that illustrate how subsurface microbial activity influences the content of produced water.

Under prevailing anaerobic and reducing conditions, microorganisms can mobilize or sequester metals found in unconventional produced water (Gadd, 2004). Microbial enzymatic reduction carried out by chromium-, iron-, manganese-, and uranium-reducing bacteria can both mobilize and sequester metals (Vanengelen et al., 2008; García et al., 2004; Mata et al., 2002; Gauthier et al., 1992; Myers and Nealson, 1988; Lovley and Phillips, 1986). For instance, iron and manganese species go into solution when reduced, while chromium and uranium species precipitate when reduced (Gadd, 2004; Newman, 2001; Ahmann et al., 1994).

Metals can also be microbially solubilized by complexing with extracellular metabolites, siderophores (metal-chelating compounds), and microbially generated bioligands (e.g., organic acids) (Glorius et al., 2008; Francis, 2007; Gadd, 2004; Hernlem et al., 1999). For example, *Pseudomonas* spp. secrete acids that act as bioligands to form complexes with uranium(VI) (Glorius et al., 2008).

Many sulfur-cycling taxa have been found in hydraulic fracturing flowback and produced water communities (Murali Mohan et al., 2013b; Mohan et al., 2011). Immediately following injection, microbial sulfate reduction is stimulated by diluting high-salinity formation waters with fresh water (high salinities inhibit sulfate reduction). Microbial sulfate reduction oxidizes organic matter and decreases aqueous sulfate concentrations, thereby increasing the solubility of barium (Cheung et al., 2010; Lovley and Chapelle, 1995).

Sulfidogens also reduce sulfate, as well as elemental sulfur and other sulfur species (e.g., thiosulfate) prevalent in the subsurface, contributing to biogenic sulfide or hydrogen sulfide gas in produced water (Alain et al., 2002; Ravot et al., 1997). Sulfide can also sequester metals in sulfide phases (Ravot et al., 1997; Lovley and Chapelle, 1995). Sources of sulfide also include formation solids (e.g., pyrite in shale) and remnants of drilling muds (e.g., barite and sulfonates), or other electron donor sources (Davis et al., 2012; Kim et al., 2010; Collado et al., 2009; Grabowski et al., 2005).

Additionally, anaerobic hydrocarbon oxidizers associated with shale produced water can readily degrade simple and complex carbon compounds across a considerable salinity and redox range (Murali Mohan et al., 2013b; Fichter et al., 2012; Timmis, 2010; Lalucat et al., 2006; Yakimov et al., 2005; McGowan et al., 2004; Hedlund et al., 2001; Cayol et al., 1994; Gauthier et al., 1992; Zeikus et al., 1983).

Lastly, microbial fermentation produces organic acids, alcohols, and gases under anaerobic conditions, as is the case during methanogenesis. Some nitrogen-cycling genera have been identified in unconventional shale gas systems. These include genera involved in nitrate reduction and denitrification (Kim et al., 2010; Yoshizawa et al., 2010; Yoshizawa et al., 2009; Lalucat et al., 2006). These genera likely couple sugar, organic carbon, and sulfur species oxidation to nitrate reduction and denitrification processes.

Consequently, using a variety of recurring physiologies, microorganisms mobilize and sequester constituents in and out of solution to influence the content of flowback and produced water in important ways.

E.3. Produced Water Content Spatial Trends

E.3.1. Variability between Plays of the Same Rock Type

E.3.1.1. Shale Formation Variability

The content of shale produced water varies geographically, as shown by data from four formations (the Bakken, Barnett, Fayetteville, and Marcellus Shales; see Table E-2, Table E-4, Table E-6, Table E-9, Table E-10). For several constituents, variability between shale formations is common. The average/median TDS concentrations in the Marcellus (87,800 to 106,390 mg/L) and Bakken (196,000 mg/L) Shales are one order of magnitude greater than the average TDS concentrations reported for the Barnett and Fayetteville Shales (see Table E-2). As Fayetteville produced water contains the lowest reported average TDS concentration (13,290 mg/L), average concentrations for many inorganics (i.e., bromide, calcium, chloride, magnesium, sodium, and strontium) that contribute to dissolved solids loads are the lowest compared to average concentrations for the same inorganics in Bakken, Barnett, and Marcellus produced water (see Table E-4 and Table E-6). Average concentrations for metals reported within Bakken and Marcellus produced water are also higher than those within the Barnett or Fayetteville formations (see Table E-6).

Additionally, Marcellus produced water is enriched in barium (average concentration of 2,224 mg/l in Barbot et al. (2013) or median calculated from Hayes (2009) of 542.5 mg/L) and strontium (average concentration of 1,695 mg/L (Barbot et al., 2013) or median calculated from Hayes (2009)of 1,240 mg/L) by one to three orders of magnitude compared to Bakken, Barnett, and Fayetteville produced water (see Table E-6). Subsequently, radionuclide variability expressed as isotopic ratios (e.g., radium-228/radium-226, strontium-87/strontium-86) are being used to determine the reservoir source for produced water (Chapman et al., 2012; Rowan et al., 2011; Blauch et al., 2009). Lastly, Barnett and Bakken produced waters are enriched in sulfate.

Although organic data are limited, average BTEX concentrations are higher in Marcellus compared to Barnett produced water by one order of magnitude, whereas concentrations of benzene alone are marginally higher in Barnett compared to Marcellus produced water (see Table E-9 and Table E-10).

E.3.1.2. Tight Formation Variability

The average concentrations for various constituents in tight formation produced water vary geographically between sandstone formations (the Cotton Valley Group, Devonian sandstone, and the Mesaverde and Oswego), as shown in Table E-2, Table E-4, and Table E-6. The average TDS concentrations in the Devonian sandstone (235,125 mg/L) and Cotton Valley Group (164,683 mg/L) are one to two orders of magnitude greater than the average TDS concentrations reported for the Mesaverde (15,802 mg/L) and Oswego Formations (73,082 mg/L) (see Table E-2).

Mesaverde produced water also contained the lowest average concentrations for many of the inorganic components of TDS (i.e., calcium, chloride, iron, magnesium, and sodium; see Table E-4 and Table E-6).

Little variability was reported in pH between these four tight formations (see Table E-2). Mesaverde produced water was enriched in sulfate, with an average concentration of 837 mg/L (see Table E-4), whereas Devonian produced water was enriched in barium, which had an average concentration of 1,488 mg/L (see Table E-6).

E.3.1.3. Coalbed Variability

Geochemical analysis showed that the Powder River Basin is predominately characterized by bicarbonate water types with a large intrusion of sodium-type waters across a large range of magnesium and calcium concentrations (Dahm et al., 2011).[1] In contrast, the Raton Basin is typified by sodium-type waters with low calcium and magnesium concentrations. A combination of Powder River and Raton produced water compositional characteristics typifies the San Juan Basin (Dahm et al., 2011). Lastly, Black Warrior Basin produced water is differentiated based upon its sodium bicarbonate- or sodium chloride-type waters (DOE, 2014; Pashin et al., 2014).

Regional variability is observed in average produced water concentrations for various constituents of four CBM basins (Powder River, Raton, San Juan, and Black Warrior; see Table E-3, Table E-5, Table E-7, Table E-9, and Table E-11), but particularly between produced water of the Black Warrior Basin and the others. As the average TDS concentration in Black Warrior Basin produced water (14,319 mg/L) is one to two orders of magnitude higher than that of the other three presented in Table E-3, average concentrations for TDS contributing ions (i.e., calcium, chloride, and sodium) were also higher than in the Powder River, Raton, and San Juan Basins. These high levels follow from the marine depositional environment of the Black Warrior Basin (Horsey, 1981).

Powder River Basin produced water has the lowest average TDS concentration (997 mg/L), which is consistent with Dahm et al. (2011) reporting that nearly a quarter of all the produced water sampled from the Powder River Basin meets the U.S. drinking water secondary standard for TDS (less than 500 mg/L).[2] In addition, the Black Warrior Basin appears to be slightly enriched in barium, compared to the other three CBM basins (see Table E-5). Lastly, the three western CBM basins (Powder River, Raton, and San Juan) are much more alkaline and enriched in bicarbonate than their eastern counterpart (the Black Warrior Basin; see Table E-3).

[1] Water is classified as a "type" if the dominant dissolved ion is greater than 50% of the total. A sodium-type water contains more that 50% of the cation milliequivalents (mEq) as sodium. Similarly, a sodium-bicarbonate water contains 50% of the cation mEq as sodium, and 50% of the anion mEq as bicarbonate (USGS, 2002).

[2] MCL refers to the highest level of a contaminant that is allowed in drinking water. MCLs are enforceable standards. These include primary MCLs for barium, cadmium, chromium, lead, mercury, and selenium. National Secondary Drinking Water Regulations (NSDWRs or secondary standards) are non-enforceable guidelines regulating contaminants that may cause cosmetic effects (such as skin or tooth discoloration) or aesthetic effects (such as taste, odor, or color) in drinking water. Secondary MCLs are recommended for aluminum, chloride, copper, iron, manganese, pH, silver, sulfate, TDS, and others. See http://water.epa.gov/drink/contaminants/index.cfm#Primary for more information.

Average concentrations of benzene, ethylbenzene, and xylenes are higher in San Juan compared to Raton produced water by two orders of magnitude, whereas concentrations of toluene are marginally higher in Raton compared to San Juan produced water (see Table E-9).

E.3.2. Local Variability

Spatial variability of produced water content frequently exists within a single producing formation. For instance, Marcellus Shale barium levels increase along a southwest to northeast transect (Barbot et al., 2013). Additionally, produced water from the northern and southern portions of the San Juan Basin differ in TDS, due to ground water recharge in the northern basin leading to higher chloride concentrations than in the southern portion (Dahm et al., 2011; Van Voast, 2003).

Spatial variability of produced water content also exists at a local level due to the stratigraphy surrounding the producing formation. For example, deep saline aquifers, if present in the over- or underlying strata, may over geologic time encroach upon shales, coals, and sandstones via fluid intrusion processes (Blauch et al., 2009). Evidence of deep brine migration from adjacent strata into shallow aquifers via natural faults and fractures has been noted previously in the Michigan Basin and the Marcellus Shale (Vengosh et al., 2014; Warner et al., 2012; Weaver et al., 1995). By extension, in situ hydraulic connectivity, which is stimulated by design during hydraulic fracturing, may lead to the migration of brine-associated constituents in under- and overlying strata into producing formations, as discussed in Chapter 6.

As hydrocarbon source rocks often form repeating sedimentary sequences, contact between these layers presents opportunities for an exchange of organics and inorganics (Fredrickson and Balkwill, 2006; U.S. EPA, 2004). For instance, diffusion of carbon sources and electron donors occurs at subsurface shale-sandstone interfaces, suggesting a stratigraphic role in the exchange of constituents between formations (Fredrickson and Balkwill, 2006).

E.4. Example Calculation for Roadway Transport

This section provides background information for the roadway transport calculation appearing in Chapter 7.

E.4.1. Estimation of Transport Distance

In a study of wastewater management for the Marcellus Shale, Rahm et al. (2013) used data reported to the Pennsylvania Department of Environmental Protection (PA DEP) to estimate the average distance wastewater was transported. For the period from 2008 to 2010, the distance transported was approximately 100 km, but it was reduced by 30% for 2011. The reduction was attributed to increased treatment infrastructure in Lycoming County, an area of intensive hydraulic fracturing operations in northeastern Pennsylvania. For the part of Pennsylvania within the Susquehanna River Basin, Gilmore et al. (2013) estimated the likely transport distances for drilling waste to landfills (256 km or 159 mi); produced water to disposal wells (388 km or 241 mi); and commercial wastewater treatment plants (CWTPs) (158 km or 98 mi). These distances are longer

than the values from Rahm et al. (2013), in part, because wells in the Susquehanna Basin are further to the east of Ohio disposal wells and some CWTPs.

E.4.2. Estimation of Wastewater Volumes

In an example water balance calculation, Gilmore et al. (2013) used 380,000 gal of flowback as the volume transported to CWTPs, 450,000 gal of flowback transported to injection wells, and 130,000 gal of un-reusable treated water also transported to injection wells for a total estimated wastewater volume of 960,000 gal per well.

E.4.3. Estimation of Roadway Accidents

The U.S. Department of Transportation (DOT) published statistics on roadway accidents (U.S. Department of Transportation, 2012) which indicate that the combined total of combination truck crashes in 2012 was 179,736, or 110 per 100 million vehicle miles (1.77 million km) (see Table E-12). As an indicator of the uncertainty of these data, DOT reported 122,240 large truck crashes from a differing set of databases (see Table E-13), with a rate of 75 per 100 million vehicle miles, which is 68% of the number of combination truck crashes.

Table E-12. Combination truck crashes in 2012 for the 2,469,094 registered combination trucks, which traveled 163,458 million miles (U.S. Department of Transportation, 2012).[a]

Type of crash	Combination trucks involved in crashes	Rates per 100 million vehicle miles traveled by combination trucks
Property damage only	135,000	82.8
Injury	42,000	25.5
Fatal	2,736	1.74
Total	179,736	110

[a] A combination truck is defined as a truck tractor pulling any number of trailers (U.S. Department of Transportation, 2012).

Table E-13. Large truck crashes in 2012 (U.S. Department of Transportation, 2012).[a]

Type of crash	Total crashes	Large trucks with cargo tanks	
		Number	Percentage
Towaway crashes	72,644	4,364	6.0%
Injury	45,794	3,245	7.1%
Fatal	3,802	360	9.5%
Totals	122,240	7,969	6.5%

[a] A large truck is defined as a truck with a gross vehicle weight rating greater than 10,000 pounds (U.S. Department of Transportation, 2012).

E.4.4. Estimation of Material Release Rates in Crashes

Estimates ranging from 5.6% to 36% have been made for the probability of material releases from crashed trucks. Craft (2004) used data from three databases to estimate the probability of spills in fatality accidents at 36%, which may overestimate the probability for all types of accidents (Rozell and Reaven, 2012).[1] The U.S. Department of Transportation (2012) provides estimates of hazardous materials releases from large truck crashes. For all types of hazardous materials carried, 408 of 2,903 crashes, or 14%, were known to have hazardous materials releases. The occurrence of a release was unknown for 18% of the crashes. These crashes were not distinguished by truck type, so they likely overestimated the number of tanker crashes. Harwood et al. (1993) used accident data from three states (California, Illinois, and Michigan) to develop hazardous materials release rate estimates for different types of roadways, accidents, and settings (urban or rural). For roadways in rural settings the probability of release ranged from 8.1% to 9.0%, while in urban settings the probability ranged from 5.6% to 6.9%.

E.4.5. Estimation of Volume Released in Accidents

Based on the estimated volume (960,000 gal (3.63 million L) per well) and disposal distances used by Rahm et al. (2013) and Gilmore et al. (2013), and an assumed 20,000 L (5,300 gal)-containing truck (Gilmore et al., 2013), the total travel distance by trucks ranges from 9,620 miles (14,900 km) to 17,760 miles (28,570 km) per well (see Table E-14).

[1] The three databases were the Trucks Involved in Fatal Accidents developed by the Center for National Truck Statistics at the University of Michigan, the National Automotive Sampling System's General Estimates System (GES) produced by the National Highway Transportation Safety Agency, and the Motor Carrier Management Information System (MCMIS) Crash File produced by the Federal Motor Carrier Safety Administration.

Table E-14. Estimate of total truck-travel miles per well in the Susquehanna River Basin based on the transport analysis performed by Gilmore et al. (2013).

Action	Waste per well (million gal)	Trucks (20 m^3/truck)	Miles traveled per truck	Total miles traveled (per well)	Material release rate bounds			
					5.6%		36%	
					Crashes per 100 million miles			
					75	110	75	110
Gilmore et al. (2013) distance estimates								
Produced water to CWTP	0.38	72	26.9	1,937				
Produced water to disposal well	0.45	85	147	12,495				
CWTP effluent to disposal well	0.13	25	133	3,325				
Total	0.96	182		17,757	3	4	18	27
Rahm et al. (2013) distance estimates								
Transport 100 km	0.96	182	62.1	11,300	2	3	12	17
Transport 70 km	0.96	182	43.5	9,620	1	2	8	12

The Susquehanna River Basin Commission reported 1,928 well pads permitted within the basin (SRBC, 2012). Assuming two wells per pad, the total distance traveled to haul hydraulic fracturing wastewater is 68.4 million miles (110 million km).

Combining these data with the DOT crash data gives an estimated 76 crashes per year using the combination truck crash rate or 52 per year using the DOT large truck crash rate. Based on the various assumptions of travel distances, crash rates, and estimated minimum and maximum material release rates, the number of crashes with releases ranges from 1 to 27 (see Table E-14).

Several limitations are inherent in this analysis, including differing rural road accident rates and highway rates, differing wastewater endpoints, and differing amounts of produced water transport. Further, the estimates present an upper bound on impacts, because not all releases of wastewater would reach or impact drinking water resources.

E.5. References for Appendix E

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Appendix F

Wastewater Treatment and Waste Disposal Supplemental Information

Appendix F. Wastewater Treatment and Waste Disposal Supplemental Information

This appendix provides additional information for context and background to support the discussions of hydraulic fracturing wastewater management and treatment in Chapter 8 of the Hydraulic Fracturing Drinking Water Assessment. Information in this appendix includes: estimates compiled for several states for volumes of wastewater generated in regions where hydraulic fracturing is occurring; an overview of the technologies that can be used to treat hydraulic fracturing wastewater; calculations of estimated treatment process effluent concentrations for example constituents; a description of the different discharge options for centralized waste treatment plants; and the water quality needed for wastewater to be reused for hydraulic fracturing. Discussion is also provided on difficulties that can arise during treatment of hydraulic fracturing wastewaters: the potential impacts of hydraulic fracturing wastewater on biological treatment processes; and an overview of the formation of disinfection byproducts.

F.1. Estimates of Wastewater Production in Regions where Hydraulic Fracturing is Occurring

Table F-1 presents estimated wastewater volumes for several states in areas with hydraulic fracturing activity. These data were compiled from production data available on state databases and were tabulated by year. For California, data were compiled for Kern County, where about 95% of hydraulic fracturing is taking place (CCST, 2015). Production records from Colorado, Utah, and Wyoming include the producing formation for each well reported; data from these states were filtered to select data from formations indicated in the literature as targets for hydraulic fracturing. Data presented for these three states include statewide estimates as well as estimates for selected basins. Data from New Mexico are available from the states in files for three basins as well as for the state; these data were not filtered further.

Results in Table F-1 illustrate some of the challenges associated with obtaining estimates of hydraulic fracturing wastewater volumes, especially using publicly available data. Some of the values likely include reported values from conventional wells (wells that may not be hydraulically fractured, and are typically not subject to modern, high volume hydraulic fracturing). For example, the well counts for California, Colorado, Utah, and Wyoming were in the thousands or tens of thousands at least as early as 2000, several years before the surge of modern hydraulic fracturing began in the mid-2000s. The data used for California were from Kern County but are not specific to hydraulic fracturing activity. Where producing formations are provided, the accuracy of the estimates will depend upon correct selection of hydraulically fractured formations. Thus, both underestimation and overestimation may be possible because of a lack of clear indication of which wells were hydraulically fractured.

Table F-1. Estimated volumes (millions of gallons) of wastewater based on state data for selected years and numbers of wells producing fluid.

State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
California	San Joaquin[a]	Shale, unconsoli-dated sands	Produced water	46,000	48,000	58,000	65,000	71,000	75,000	74,000	-	Data from CA Department of Conservation, Oil and Gas Division.[a] Produced water data compiled for Kern County. Data may also represent contributions from production without hydraulic fracturing.
			Wells	*33,695*	*39,088*	*46,519*	*49,201*	*51,031*	*51,567*	*52,763*	-	
Colorado	All basins with hy-draulically fractured formations	-	Produced water	7,300	11,000	21,000	14,000	12,000	12,000	7,700	-	Data from CO Oil and Gas Conservation Commission.[b] Produced water includes flowback. Data filtered for formations indicated in literature as undergoing hydraulic fracturing and matched to corresponding basins. Example counties selected for presentation as well as estimated state total.
			Wells	*11,264*	*14,934*	*28,282*	*33,929*	*35,999*	*38,371*	*37,618*	-	
	Denver	Sandstone, shale	Produced water	140	160	170	160	160	150	110	-	
			Wells	*1,829*	*1,511*	*1,277*	*1,204*	*1,193*	*1,131*	*1,072*	-	
	Piceance	Sandstone	Produced water	3,500	5,800	9,300	6,900	6,500	6,800	4,300	-	
			Wells	*1,134*	*2,478*	*6,486*	*9,105*	*10,057*	*10,868*	*10,954*	-	

State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
Colorado, cont.	Raton	Coalbed methane	Produced water	2,400	4,100	8,900	4,300	3,200	2,700	2,100	-	
			Wells	*681*	*1,634*	*2,795*	*2,734*	*2,778*	*2,710*	*2,545*	-	
	San Juan	Coalbed methane	Produced water	1,000	1,100	1,300	2,000	1,200	1,100	650	-	
			Wells	*1,183*	*1,605*	*1,975*	*2,220*	*2,308*	*2,328*	*2,333*	-	
New Mexico	Permian	Shale, sandstone	Produced water	-	-	-	-	-	31,000	31,000	20,000	Data from New Mexico Oil Conservation Division.[c] Data provided by the state by basin and for the entire state. Unclear how much contribution from production without hydraulic fracturing. Produced water includes flowback.
			Wells	-	-	-	-	-	*29,839*	*30,386*	*30,287*	
	Raton	Coalbed methane	Produced water	-	-	-	-	-	510	540	310	
			Wells	-	-	-	-	-	*1,495*	*1,502*	*1,526*	
	San Juan	Coalbed methane	Produced water	-	-	-	-	-	1,700	2,000	1,100	
			Wells	-	-	-	-	-	*22,492*	*22,349*	*22,076*	
	Total	-	Produced water	-	-	-	-	-	33,000	34,000	22,000	
			Wells	-	-	-	-	-	*53,826*	*54,237*	*53,889*	

State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
Utah	All basins with hydraulically fractured formations	-	Produced water	1,200	1,200	2,300	2,400	2,700	2,900	3,400	2,800	Data from State of Utah Oil and Gas Program.[d] Produced water includes flowback. Data filtered by formation indicated in the literature as hydraulically fractured and matched to basins. Data presented for selected basins as well as for all formations likely to be hydraulically fractured.
			Wells	*3,080*	*4,377*	*7,409*	*8,432*	*9,101*	*10,075*	*10,661*	*10,900*	
	Kaiparowits/ Uinta	Coalbed methane	Produced water	860	740	1,300	1,400	1,800	2,000	2,400	1,900	
			Wells	*1,718*	*2,517*	*3,761*	*4,329*	*4,838*	*5,538*	*6,046*	*6,334*	
	San Juan/ Uinta	Coalbed methane	Produced water	2	49	350	270	240	230	190	120	
			Wells	*62*	*223*	*910*	*933*	*959*	*951*	*867*	*870*	
	Uinta	Shale/sandstone	Produced water	350	420	560	680	700	640	830	790	
			Wells	*1,067*	*1,396*	*2,282*	*2,745*	*2,888*	*3,115*	*3,257*	*3,223*	
Wyoming	All basins with hydraulically fractured formations	-	Produced water	1,300	1,400	1,300	1,500	1,600	1,700	1,600	1,800	Data from Wyoming Oil and Gas Conservation Commission.[e] Produced water may include flowback. Data filtered by formation indicated in the literature as hydraulically fractured and matched to basins. Data presented for selected basins as well as for all formations likely to be hydraulically fractured.

State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
Wyoming, cont.			*Wells*	*3,470*	*3,378*	*3,585*	*3,620*	*3,728*	*3,843*	*4,030*	*4,213*	
	Big Horn	Sandstone	Produced water	380	350	350	380	430	440	420	440	
			Wells	*365*	*359*	*387*	*397*	*412*	*414*	*407*	*403*	
	Denver	Sandstone	Produced water	54	44	49	59	76	90	97	170	
			Wells	*142*	*118*	*124*	*140*	*167*	*204*	*230*	*278*	
	Green River	Sandstone/ shale	Produced water	0	1	2	8	5	5	9	15	
			Wells	*44*	*44*	*60*	*67*	*67*	*59*	*64*	*67*	
	Powder River	Coalbed methane	Produced water	690	630	620	660	700	840	970	1,100	
			Wells	*1,953*	*1,900*	*2,001*	*2,028*	*2,119*	*2,207*	*2,352*	*2,565*	
	Wind River/ Powder River	Sandstone/ shale	Produced water	130	330	330	400	420	290	110	41	
			Wells	*966*	*957*	*1,013*	*988*	*963*	*959*	*977*	*900*	

[a] California Department of Conservation, Oil and Gas Division. Oil & Gas – Online Data. Monthly Production and Injection Databases: ftp://ftp.consrv.ca.gov/pub/oil/new_database_format/.

[b] Colorado Oil and Gas Conservation Commission. Data: Downloads: Production Data: http://cogcc.state.co.us/data2.html#/downloads.

[c] New Mexico Oil Conservation Division. Production Data. Production Summaries: All Wells Data: http://gotech.nmt.edu/gotech/Petroleum_Data/allwells.aspx.

[d] Utah Department of Natural Resources. Division of Oil, Gas, and Mining. Data Research Center. Database Download Files: http://oilgas.ogm.utah.gov/Data_Center/DataCenter.cfm#production.

[e] Wyoming Oil and Gas Conservation Commission. Production files by county and year: http://wogcc.state.wy.us/productioncountyyear.cfm?Oops=#oops#&RequestTimeOut=6500.

F.2. Overview of Treatment Processes for Treating Hydraulic Fracturing Wastewater

Treatment technologies discussed in this appendix are classified as basic or advanced. Basic treatment technologies are ineffective for reducing total dissolved solids (TDS) and are typically not labor intensive. Advanced treatment technologies can remove TDS and/or are complex in nature (e.g., energy- and labor-intensive).

F.2.1. Basic Treatment

Basic treatment technologies include physical separation, coagulation/oxidation, electrocoagulation, sedimentation, and disinfection. These technologies are effective at removing total suspended solids (TSS), oil and grease, scale-forming compounds, and metals, and they can minimize microbial activity. Basic treatment is typically incorporated in a permanent treatment facility (i.e., fixed location) but can also be part of a mobile unit for onsite treatment applications.

F.2.1.1. Physical Separation

The most basic treatment need for oil and gas wastewaters, including those from hydraulic fracturing operations, is separation to remove suspended solids, and oil and grease. The separation method largely depends on the type of resource(s) targeted by the hydraulic fracturing operation. Down-hole separation techniques, including mechanical blocking devices and water shut-off chemicals to prevent or minimize water flow to the well, may be used during production in shale plays containing greater amounts of liquid hydrocarbons. To treat water at the surface, separation technologies such as hydrocyclones, dissolved air or induced gas flotation systems, media (sand) filtration, and biological aerated filters can remove suspended solids and some organics from hydraulic fracturing wastewater.

Media filtration can also remove hardness and some metals if chemical precipitation (i.e., coagulation, lime softening) is also employed (Boschee, 2014). An example of a centralized waste treatment facility (CWT) that uses chemical precipitation and media filtration to treat hydraulic fracturing waste is the Water Tower Square Gas Well Wastewater Processing Facility in Pennsylvania (see Table 8-7). One or more of these technologies is typically used prior to advanced treatment such as reverse osmosis (RO) because advanced treatment processes foul, scale, or otherwise do not operate effectively in the presence of TSS, certain organics, and/or some metals and metalloid compounds (Boschee, 2014; Drewes et al., 2009). The biggest challenge associated with use of these separation technologies is solids disposal from the resulting sludge (Igunnu and Chen, 2014).

F.2.1.2. Coagulation/Oxidation

Coagulation is the process of agglomerating small, unsettleable particles into larger particles to promote settling. Chemical coagulants such as alum, iron chloride, and polymers can be used to precipitate TSS, some dissolved solids (except monovalent ions such as sodium and chloride), and metals from hydraulic fracturing wastewater. Adjusting the pH using chemicals such as lime or caustic soda can increase the potential for some constituents, including dissolved metals, to form precipitates. Chemical precipitation is often used in industrial wastewater treatment as a

pretreatment step to decrease the pollutant loading on subsequent advanced treatment technologies; this strategy can save time, money, energy consumption and the lifetime of the infrastructure.

Processes using advanced oxidation and precipitation have been applied to hydraulic fracturing wastewaters in on-site and mobile systems. Hydroxyl radicals generated by cavitation processes and the addition of ozone can degrade organic compounds and inactivate micro-organisms. The process can also aid in the precipitation of elements, which cause hardness and scaling in the treated water (e.g. calcium, magnesium). The process can also reduce sulfate and carbonate concentrations in the treated water. This type of treatment can be very effective for on-site reuse of wastewater (Ely et al., 2011).

The produced solid residuals from coagulation/oxidation processes typically require further treatment, such as de-watering (Duraisamy et al., 2013; Hammer and VanBriesen, 2012).

F.2.1.3. Electrocoagulation

Electrocoagulation (EC) (Figure F-1) combines the principles of coagulation and electrochemistry into one process (Gomes et al., 2009). An electrical current added to the wastewater produces coagulants that then neutralize the charged particles, causing them to destabilize, precipitate, and settle. EC may be used in place of, or in addition to, chemical coagulation. EC can be effective for removal of organics, TSS, and metals, but it is less effective for removing TDS and sulfate. Although it is still considered an emerging technology for unconventional oil and gas wastewater treatment, EC has been used in mobile treatment systems to treat hydraulic fracturing wastewaters (Halliburton, 2014; Igunnu and Chen, 2014). Limitations with this technology are the potential for scaling, corrosion, and bacterial growth (Gomes et al., 2009).

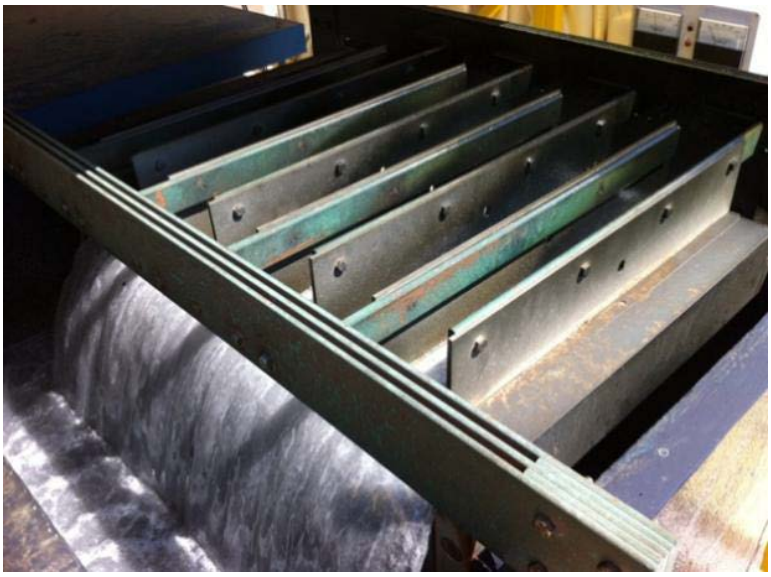

Figure F-1. Electrocoagulation unit.

Source: Dunkel (2013).

F.2.1.4. Sedimentation

Treatment plants may include sedimentation tanks, clarifiers, or some other form of settling basin to allow larger particles to settle out of the water where they can eventually be collected, dewatered, and disposed of. These types of tanks/basins all serve the same purpose – to reduce the amount of solids going to subsequent processes (i.e., overload the media filters).

F.2.1.5. Disinfection

Some hydraulic fracturing applications may require disinfection to kill bacteria after treatment and prior to reuse. Chlorine is a common disinfectant. Chlorine dioxide, ozone, or ultraviolet light can also be used. This is an important step for reused water because bacteria can cause problems for further hydraulic fracturing operations by multiplying rapidly and causing build-up in the well bore, which decreases gas extraction efficiency.

F.2.2. Advanced Treatment

Advanced treatment technologies consist of membranes (reverse osmosis (RO), nanofiltration, ultrafiltration, microfiltration, electrodialysis, forward osmosis, and membrane distillation), thermal distillation technologies, crystallizers, ion exchange, and adsorption. These technologies are effective for removing TDS and/or targeted compounds. They typically require pretreatment to remove solids and other constituents that may damage or otherwise impede the technology from operating as designed. Advanced treatment technologies can be energy intensive and are typically employed when a purified water effluent is necessary for direct discharge, indirect discharge, or reuse. In some instances, these water treatment technologies can make use of methane generated by the gas well as an energy source. Some advanced treatment technologies can be made mobile for on-site treatment.

F.2.2.1. Membranes

Pressure-driven membrane processes including microfiltration, ultrafiltration, nanofiltration, and RO (Figure F-2) are being used in some settings to treat oil and gas wastewater. These processes use hydraulic pressure to overcome the osmotic pressure of the influent waste stream, forcing clean water through the membrane (Drewes et al., 2009). Microfiltration and ultrafiltration processes do not reduce TDS but can remove TSS and some metals and organics (Drewes et al., 2009). RO and nanofiltration are capable of removing TDS, including anions and radionuclides. RO, however, may be limited to treating TDS levels of approximately 40,000 mg/L TDS (Shaffer et al., 2013; Younos and Tulou, 2005).

Figure F-2. Photograph of reverse osmosis system.

Source: Thinkstock.

F.2.2.2. Electrodialysis

Electrodialysis relies on positively and negatively charged particles and coated membranes to separate contaminants from the water (Figure F-3). Electrodialysis has been considered for use by the shale gas industry, but it is not currently widely utilized (ALL Consulting, 2013). TDS concentrations above 15,000 mg/L are difficult to treat by electrodialysis (ALL Consulting, 2013), and oil and divalent cations (e.g. Ca, Fe, Mg) can foul the membranes (Hayes and Severin, 2012b; Guolin et al., 2008).

Figure F-3. Picture of mobile electrodialysis units in Wyoming.

Source: DOE (2006). Permission: ALL Consulting.

F.2.2.3. Forward Osmosis/Membrane Distillation

Forward osmosis, an emerging technology for treating hydraulic fracturing wastewater, uses an osmotic pressure gradient across a membrane to draw the contaminants from a low osmotic solution (the feed water) to a high osmotic solution (Drewes et al., 2009). The selection of the constituents for the draw solution is very important as the constituents should be more easily removed from solution than the compounds (e.g. salts) in the feed. Alternatively, draw solutions can contain components that are more easily reused or recycled. Another emerging technology, membrane distillation, relies on a thermal gradient across a membrane surface to volatilize pure water and capture it in the distillate (Drewes et al., 2009).

F.2.2.4. Thermal Distillation

Thermal distillation technologies, such as mechanical vapor recompression (MVR) (Figure F-4) and dewvaporation, use liquid-vapor separation by applying heat to the waste stream, vaporizing the water to separate out impurities, and condensing the vapor into distilled water (Drewes et al., 2009; LEau LLC, 2008; Hamieh and Beckman, 2006). MVR and dewvaporation can treat high-TDS waters and have been proven in the field as effective for treating oil and gas wastewater (Hayes and Severin, 2012b; Drewes et al., 2009). Like RO, these processes are energy intensive and are used when the objective is very clean water (i.e., TDS less than 500 mg/L) for direct/indirect discharge or if clean water is needed for reuse. As with membrane processes, scaling is an issue with these technologies, and scale inhibitors may be needed for them to operate effectively (Igunnu and Chen, 2014).

Figure F-4. Picture of a mechanical vapor recompression unit near Decatur, Texas.

Source: Drewes et al. (2009). Permission provided.

CWTs such as the Judsonia Central Water Treatment Facility in Arkansas, and the Casella-Altela Regional Environmental Services and Clarion Altela Environmental Services, both in Pennsylvania, have NPDES permits and use MVR or thermal distillation for TDS removal. Figure F-5 shows a diagram of the treatment train at another facility, the Maggie Spain facility in Texas, which uses MVR in its treatment of Barnett Shale wastewater (Hayes and Severin, 2012a).

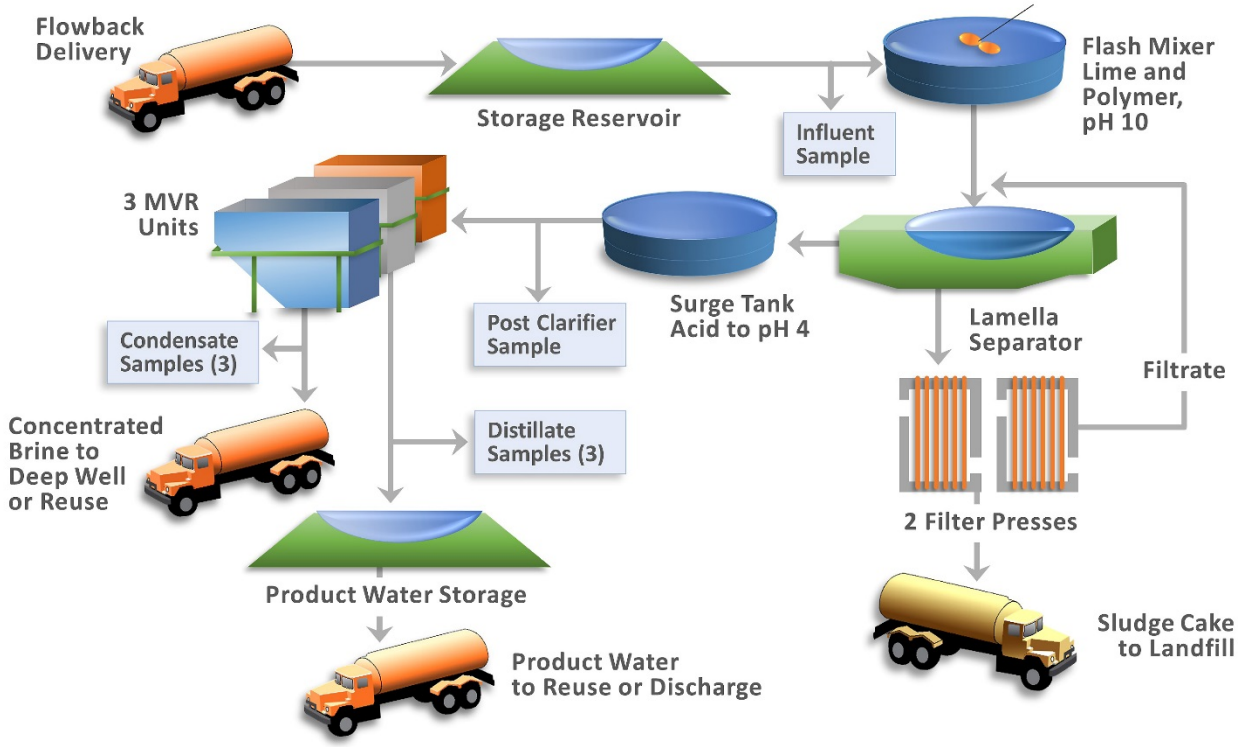

Figure F-5. Mechanical vapor recompression process design – Maggie Spain Facility.

Adapted from: Hayes and Severin (2012a).

Crystallizers can be employed at CWTs to treat high-TDS waters or to further concentrate the waste stream from a distillation process, reducing residual waste disposal volumes. The crystallized salt can be landfilled, deep-well injected, or used to produce pure salt products that may be salable (Ertel et al., 2013).

Another thermal method, freeze-thaw evaporation, involves spraying wastewater onto a freezing pad, allowing ice crystals to form, and the brine mixture that remains in solution to drain from the ice (Drewes et al., 2009). In warmer weather, the ice thaws and the purified water is collected. This technology cannot treat waters with high methanol concentrations and is only suitable for areas where the temperature is below freezing in the winter months (Igunnu and Chen, 2014). In addition, freeze-thaw evaporation can only reduce TDS concentrations to approximately 1,000 mg/L, which is higher than the 500 mg/L TDS surface water discharge limit required by most permits (Igunnu and Chen, 2014).

F.2.2.5. Ion Exchange and Adsorption

Ion exchange (Figure F-6) is the process of exchanging ions on a media referred to as resin for unwanted ions in the water. Ion exchange is used to treat for target ions that may be difficult to remove by other treatment technologies or that may interfere with the effectiveness of advanced treatment processes.

Figure F-6. Picture of a compressed bed ion exchange unit.

Source: Drewes et al. (2009). Permission provided.

Adsorption is the process of adsorbing contaminants onto a charged granular media surface. Adsorption technologies can effectively remove organics, heavy metals, and some anions (Igunnu and Chen, 2014). With ion exchange and adsorption processes, the type of resin or adsorptive media used (e.g., activated carbon, organoclay, zeolites) dictates the specific contaminants that will be removed from the water (Drewes et al., 2009; Fakhru'l-Razi et al., 2009).

Because they can be easily overloaded by contaminants, ion exchange and adsorption treatment processes are generally used as a polishing step following other treatment processes or as a unit process in a treatment train rather than as stand-alone treatment (Drewes et al., 2009). Stand-alone units require more frequent regeneration and/or replacement of the spent media making these technologies more costly to operate (Igunnu and Chen, 2014). Figure F-7 shows a schematic of the Pinedale Anticline Water Reclamation Facility located in Wyoming, which uses an ion exchange unit with boron-selective resin as a polishing step to treat hydraulic fracturing wastewater specifically for boron (Boschee, 2012).

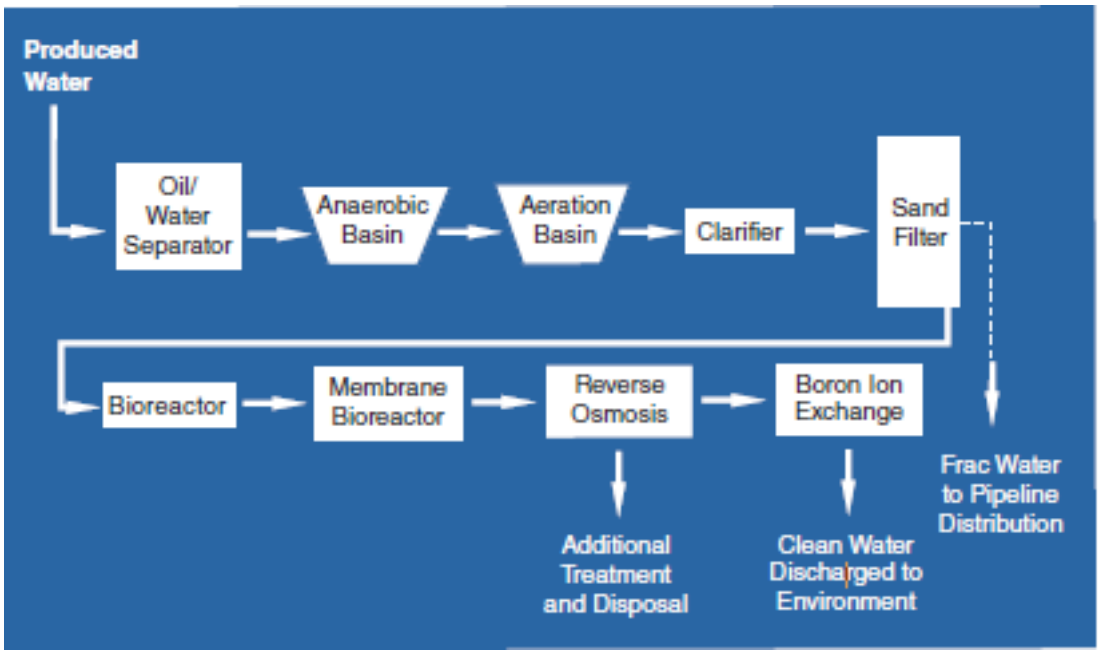

Figure F-7. Discharge water process used in the Pinedale Anticline field.

Source: Boschee (2012).

F.3. Treatment Technology Removal Capabilities

Table F-2 provides removal efficiencies for common hydraulic fracturing wastewater constituents by treatment technology. With the exception of TSS and TDS, the studies cited demonstrate removal for a subset of constituents in a category (e.g., Gomes et al., 2009) reported that electrodialysis was an effective treatment for oil and grease, not all organics). The removal efficiencies include ranges of 1 to 33% (denoted by +), 34% to 66% (denoted by ++), and greater than 66% removal (denoted by +++). Cells denoted with "--" indicate that the treatment technology is not suitable for removal of that constituent or group of constituents. If a particular treatment technology only lists removal efficiencies for TDS, it can be assumed that in some cases, cations and anions would also be removed by that technology; therefore, where specific results were not provided in literature, cells denoted with "Assumed" refer to cations and anions that comprise TDS.

Table F-2. Removal efficiency of different hydraulic fracturing wastewater constituents using various wastewater treatment technologies.[a]

Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Hydrocyclones	+++ (Duraisamy et al., 2013)	--	--	--	--	++ (Duraisamy et al., 2013)
Evaporation (freeze-thaw evaporation)	+++ (Igunnu and Chen, 2014; Drewes et al., 2009)	+++ (Igunnu and Chen, 2014; Drewes et al., 2009; Arthur et al., 2005)	Assumed	+++ (Igunnu and Chen, 2014; Drewes et al., 2009; Arthur et al., 2005)	--	+++ (Igunnu and Chen, 2014; Duraisamy et al., 2013; Drewes et al., 2009)
Filtration (granular media)	+++ (Barrett, 2010)	--	--	+++[b] (Duraisamy et al., 2013)	--	+++ (Shafer, 2011; Drewes et al., 2009)
Chemical precipitation	+++ (Fakhru'l-Razi et al., 2009)	--	--	+++ (Fakhru'l-Razi et al., 2009; AWWA, 1999)	+++[c] (Zhang et al., 2014)	+++ (Fakhru'l-Razi et al., 2009)
Sedimentation (clarifier)	++ (NMSU DACC WUTAP, 2007)	--	--	--	--	--
Dissolved air flotation	+++ (Shammas, 2010)	--	--	--	--	++/+++ (Duraisamy et al., 2013; Fakhru'l-Razi et al., 2009)
Electro-coagulation	+++ (Igunnu and Chen, 2014; Bukhari, 2008)	--	--	+ (Igunnu and Chen, 2014)	--	+++ (Igunnu and Chen, 2014; Duraisamy et al., 2013; Fakhru'l-Razi et al., 2009)
Advanced oxidation and precipitation	--	+ (Abrams, 2013)	--	+/+++ (Abrams, 2013)	--	+++[d] (Duraisamy et al., 2013) (Fakhru'l-Razi et al., 2009)

Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Reverse osmosis	--	++/+++[e] (Alzahrani et al., 2013; Drewes et al., 2009)	+++ (Alzahrani et al., 2013) (Arthur et al., 2005)	++/+++[f] (Alzahrani et al., 2013) (Drewes et al., 2009; AWWA, 1999)	+++ (Drewes et al., 2009)	+/++/+++[g] (Drewes et al., 2009; Munter, 2000)
Membrane filtration (UF/MF)	+++ (Arthur et al., 2005)	--	--	+++ (Fakhru'l-Razi et al., 2009)	--	++/+++ (Duraisamy et al., 2013; Fakhru'l-Razi et al., 2009; Hayes and Arthur, 2004; AWWA, 1999)[h]
Forward osmosis	--	+++ (Drewes et al., 2009)	Assumed	Assumed	--	--
Distillation, including thermal distillation (e.g., mechanical vapor recompression (MVR))		+++[i] (Hayes et al., 2014; Bruff and Jikich, 2011; Drewes et al., 2009)	+++ (Bruff and Jikich, 2011; Drewes et al., 2009)	+++ (Hayes et al., 2014; Bruff and Jikich, 2011; Drewes et al., 2009)	+++ (Bruff and Jikich, 2011; Drewes et al., 2009)	+/++/+++ (Hayes et al., 2014; Duraisamy et al., 2013; Drewes et al., 2009; Fakhru'l-Razi et al., 2009)
Ion exchange	--	--	+++ (Drewes et al., 2009)	+++ (Drewes et al., 2009; Arthur et al., 2005)	+++ (Drewes et al., 2009)	+/++/+++ (Fakhru'l-Razi et al., 2009; Munter, 2000)[j]
Crystallization	--	+++ (ER, 2014)	Assumed	Assumed	--	--
Electrodialysis	--	+++[k] (Drewes et al., 2009; Gomes et al., 2009; Arthur et al., 2005)	++/+++ (Banasiak and Schäfer, 2009)	+/++/+++ (Banasiak and Schäfer, 2009)	--	+++ (Gomes et al., 2009)
Capacitive deionization (emerging technology)	--	+++[l] (Drewes et al., 2009)	--	--	--	--

Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Adsorption[m]	--	--	+/++/+++[n] (Habuda-Stanic et al., 2014)	+++ (Igunnu and Chen, 2014; Drewes et al., 2009)	--	+/++/+++ (Arthur et al., 2005; Hayes and Arthur, 2004; Munter, 2000)
Biological treatment	+++ (Igunnu and Chen, 2014; Drewes et al., 2009)	--	--	--	--	+/++/+++ (Igunnu and Chen, 2014; Drewes et al., 2009; Fakhru'l-Razi et al., 2009)
Constructed wetland/reed beds	++/+++ (Manios et al., 2003)	+ (Arthur et al., 2005)	--	++/+++ (Fakhru'l-Razi et al., 2009)	--	+/ +++ (Fakhru'l-Razi et al., 2009; Arthur et al., 2005)

[a] To the extent possible, removal efficiencies are based on an individual treatment technology that does not assume extensive pretreatment or combined treatment processes. However, it should be noted that some processes cannot effectively operate without pretreatment (e.g., RO, media filtration, sedimentation).

[b] Pretreatment (pH adjustment, aeration, solids separation) required.

[c] Radium co-precipitation with barium sulfate.

[d] The Fenton process.

[e] Typically requires pretreatment. Not a viable technology if TDS influent >50,000 mg/L.

[f] Iron and manganese oxides will foul the membranes.

[g] Some organics will foul the membranes (e.g., organic acids).

[h] Ultrafiltration membrane was modified with nanoparticles.

[i] Can typically handle high TDS concentrations.

[j] Resin consisted of modified zeolites that targeted removal of BTEX.

[k] Influent TDS for this technology should be <8,000 mg/L.

[l] Specific technology was an electronic water purifier which is a hybrid of capacitive deionization. Influent TDS for this technology should be <3,000 mg/L.

[m] Typically polishing step, otherwise can overload bed quickly with organics.

[n] Removal efficiency is dependent on the type of adsorbent used and the water quality characteristics (e.g., pH).

Given the variety of properties among classes of organic constituents, different treatment processes may be required depending upon the types of organic compounds needing removal. Table F-3 lists treatment processes and the classes of organic compounds they can treat.

Table F-3. Treatment processes for hydraulic fracturing wastewater organic constituents.

Treatment processes	Organic compounds removed	References
Adsorption with activated carbon	Soluble organic compounds	Fakhru'l-Razi et al. (2009)
Adsorption with organoclay media	Insoluble organic compounds	Fakhru'l-Razi et al. (2009)
Aeration	Volatile organic compounds	Tchobanoglous et al. (2013)
Dissolved air flotation	Volatile organic compounds, dispersed oil	Drewes et al. (2009)
Freeze/thaw evaporation[a]	TPH, volatile organic compounds, semi-volatile organic compounds	Duraisamy et al. (2013); Drewes et al. (2009)
Ion exchange (with modified zeolites)	BTEX, chemical oxygen demand, biochemical oxygen demand	Hayes et al. (2014); Duraisamy et al. (2013); Drewes et al. (2009); Fakhru'l-Razi et al. (2009); Munter (2000)
Distillation	BTEX, polycyclic aromatic hydrocarbons (PAHs)	Hayes et al. (2014); Duraisamy et al. (2013); Drewes et al. (2009); Fakhru'l-Razi et al. (2009).
Chemical precipitation	Oil & grease	Drewes et al. (2009); Fakhru'l-Razi et al. (2009)
Chemical Oxidation	Oil & grease	Drewes et al. (2009); Fakhru'l-Razi et al. (2009)
Media filtration (walnut shell media or sand)	Oil & grease	Drewes et al. (2009); Fakhru'l-Razi et al. (2009)
Microfiltration	Oil & grease	Drewes et al. (2009); Fakhru'l-Razi et al. (2009)
Ultrafiltration	Oil & grease, BTEX	Drewes et al. (2009); Fakhru'l-Razi et al. (2009)
Reverse osmosis[b]	Dissolved organics	Drewes et al. (2009); U.S. EPA (2005)
Electrocoagulation	Chemical oxygen demand, Biochemical oxygen demand	Fakhru'l-Razi et al. (2009)
Biologically aerated filters	Oil & grease, TPH, BTEX	Fakhru'l-Razi et al. (2009)
Reed bed technologies	Oil & grease, TPH, BTEX	Fakhru'l-Razi et al. (2009)
Hydrocyclone separators	Dispersed oil	Drewes et al. (2009)

[a] Technology cannot be used if the methanol concentration in the hydraulic fracturing wastewater exceeds 5%.

[b] RO will remove specific classes of organic compounds with removal efficiencies dependent on the compound's structure and the physical and chemical properties of the hydraulically fractured wastewater. Organoacids will foul membranes.

Table F-4 presents estimated effluent concentrations that could be produced by a variety of unit treatment processes for several example constituents and for various influent concentrations. This

analysis uses treatment process removal efficiencies from literature used to develop Table F-2 and average wastewater concentrations of several constituents presented in Chapter 7 and Appendix E. These estimates were done to illustrate the combined effects of influent wastewater composition and treatment process choice on achievable effluent concentrations. The removal efficiencies represent a variety of studies, primarily at bench and pilot scale, and done with either conventional or hydraulic fracturing wastewater. Removal efficiency for a given treatment process can vary due to a number of factors, and constituent removal may be different in a full-scale facility that uses several processes. Thus, the calculations shown in Table F-4 are intended to be rough approximations for illustrative purposes.

Table F-4. Estimated effluent concentrations for example constituents based on treatment process removal efficiencies.

Shale/ Sandstone Play	Contaminant	MCL	Avg. Influent Conc.	Units	Freeze-Thaw Evaporation	Media Filtration	Chemical Precipitation			Flotation (DAF)	Electro-coagulation	Advanced Oxidation and precipitation	Reverse osmosis	Membrane Filtration (UF/MF)	Distillation			Ion exchange			Electrodialysis	Adsorption			Biological Treatment (biodisks, BAFs)			Constructed Wetland
Bakken	Barium	**2**	10	mg/L		1						0.44	0.8		0.1	-	0.3	ND	-	0.7								2.2
Barnett	Barium	**2**	3.6	mg/L		0.4						0.16	0.29		0.036	-	0.11	ND	-	0.3								0.8
Fayetteville	Barium	**2**	4	mg/L		0.4						0.18	0.32		0.04	-	0.12	ND	-	0.3								0.9
Marcellus	Barium	**2**	2200	mg/L		220						98	180		22	-	67	ND	-	160								490
Cotton Valley	Barium	**2**	160	mg/L		16						7	13		1.6	-	4.8	ND	-	11								35
Mesaverde	Barium	**2**	140	mg/L		14						6.1	11		1.4	-	4.2	ND	-	9.7								31
Marcellus	Cadmium	**5**	25	µg/L	2.5	2.5							13										5					15
Bakken	Strontium	--	760	mg/L		76									7.6	-	23	53										
Barnett	Strontium	--	530	mg/L		53									5.3	-	16	37										
Fayetteville	Strontium	--	27	mg/L		2.7									0.27	-	0.81	1.9										
Marcellus	Strontium	--	1700	mg/L		170									17	-	51	120										
Cotton Valley	Strontium	--	2300	mg/L		230									23	-	69	160										
Devonian Sandstone	Strontium	--	3900	mg/L		390									39	-	120	270										
Marcellus	Radium 226	--	620	pCi/L			32	-	440				6.2		6.2	-	19	44										

Shale/ Sandstone Play	Contaminant	MCL	Avg. Influent Conc.	Units	Freeze-Thaw Evaporation	Media Filtration	Chemical Precipitation			Flotation (DAF)	Electro-coagulation	Advanced Oxidation and precipitation	Reverse osmosis	Membrane Filtration (UF/MF)	Distillation			Ion exchange			Electrodialysis	Adsorption			Biological Treatment (biodisks, BAFs)			Constructed Wetland
Devonian Sandstone	Radium 226	--	2400	pCi/L			120	-	1700				24		24	-	71	170										
Marcellus	Radium 228	--	120	pCi/L			6.2	-	85				1.2		1.2	-	3.6	8.4										
Marcellus	Total Radium	**5**	2500	pCi/L			130	-	1800				25		25	-	76	180										
Barnett	TOC	--	9.8	mg/L										0.2								0.98	-	2.9	2.1	-	4	1
Marcellus	TOC	--	160	mg/L										3.2								16	-	48	35	-	58	16
Cotton Valley	TOC	--	200	mg/L										4								20	-	59	44	-	71	20
Barnett	BOD	--	580	mg/L							58							290	-	440					29	-	87	47
Marcellus	BOD	--	40	mg/L							4							20	-	30					2	-	6	3.2
Barnett	O&G	--	160	mg/L		16								16							8	1.6			43			9.8
Marcellus	O&G	--	74	mg/L		7.4								7.4							3.7	0.74			19			4.4
Barnett	Benzene	**5**	680	µg/L	68									310		6.8						110						ND
Marcellus	Benzene	**5**	360	µg/L	36									170		3.6						58						ND
Barnett	Toluene	**1,000**	760	µg/L	76									350								84						ND
Marcellus	Toluene	**1,000**	1100	µg/L	110									510								120						ND
Barnett	Ethylbenzene	**700**	29	µg/L	2.9					17												3.2						ND
Marcellus	Ethylbenzene	**700**	150	µg/L	15					90												17						ND
Barnett	Xylenes	**10,000**	360	µg/L	36									170								14						ND
Marcellus	Xylenes	**10,000**	1300	µg/L	130									600								52						ND
Barnett	BTEX	--	1800	µg/L	180							7.3				91		270	-	550		3.7	-	91				

Shale/ Sandstone Play	Contaminant	MCL	Avg. Influent Conc.	Units	Freeze-Thaw Evaporation	Media Filtration	Chemical Precipitation			Flotation (DAF)	Electro-coagulation	Advanced Oxidation and precipitation	Reverse osmosis	Membrane Filtration (UF/MF)	Distillation			Ion exchange			Electrodialysis	Adsorption			Biological Treatment (biodisks, BAFs)			Constructed Wetland
Marcellus	BTEX	--	2900	µg/L	290							12				150		440	-	870		5.8	-	150				
Barnett	Naphthalene	--	240	µg/L								0.95																
Marcellus	Naphthalene	--	360	µg/L								1.4																
Barnett	1,2,4-Trimethyl-benzene	--	170	µg/L								0.69																
Marcellus	1,2,4-Trimethyl-benzene	--	430	µg/L								1.7																
Barnett	1,2,4-Trimethyl-benzene	--	59	µg/L								0.24																
Marcellus	1,2,4-Trimethyl-benzene	--	310	µg/L								1.2																

ND = Non-detect

F.4. Centralized Waste Treatment Facilities and Waste Management Options

CWTs are designed to treat for site-specific wastewater constituents so that the effluent meets the requirements of the designated disposal option(s) (i.e., reuse, direct/indirect discharge). The most basic treatment processes that a CWT might use include (Easton, 2014; Duhon, 2012):

- Physical treatment technologies such as dissolved air or gas flotation technologies, media filtration, hydrocyclones, and clarification;
- Chemical treatment technologies such as chemical precipitation and chemical oxidation; and
- Biological treatment technologies such as biological aerated filter systems and reed beds.

While these technologies are effective at removing oil and grease, suspended solids, scale-forming compounds, and some heavy metals, if TDS should be reduced as required by the intended disposal option, advanced processes such as RO, thermal distillation, or evaporation are necessary.

F.4.1. Discharge Options for CWTs

Direct discharge CWTs are allowed to discharge treated wastewater directly to surface waters under the NPDES permit program. Discharge limitations may be based on water quality standards in the NPDES and technology-based effluent limitation guidelines under 40 CFR Part 437. In addition, permitting authorities have permitted facilities for discharge under 40 CFR 435, Subpart E. Judsonia Central Water Treatment Facility in Sunnydale, Arkansas is permitted to directly discharge treated effluent from produced and flowback waters from the Fayetteville Shale play to Byrd pond located on the property. Pinedale Anticline Field Wastewater Treatment Facility in Wyoming, WY, originally designed to treat produced water from tight gas plays in the Pinedale Anticline Field to levels suitable for reuse, was upgraded to include RO treatment for discharge to a local river. CWTs with NPDES discharge permits may also opt to treat oil and gas wastewater for reuse. Some facilities have the ability to treat wastewater to different qualities (e.g., with or without TDS removal), which they might do to target various reuse water quality criteria. Both the Judsonia facility and Pinedale facility discussed above have the ability to employ either TDS- or non-TDS-removal treatment depending on the customers' needs.

Indirect discharge CWTs may treat hydraulic fracturing wastewater and then discharge the treated wastewater effluent to a POTW. Discharge to the POTW is controlled by an Industrial User mechanism, which incorporates pretreatment standards established in 40 CFR Part 437. Two facilities located in Pennsylvania (Eureka Resources) and Ohio (Patriot Water Treatment) include indirect discharge as an option in wastewater treatment. The Eureka-Williamsport facility accepts wastewater (primarily from the Marcellus Shale play) and either treats it for reuse or discharges it to the local POTW. The Patriot facility offers services to hydraulic fracturing operators in the Marcellus and Utica Shale plays for removal of solids and metals using chemical treatment. As of March 2015, however, the Patriot facility is limited by the Ohio Environmental Protection Agency in accepting only "low salinity" (<50,000 mg/L TDS) produced water and may only discharge 100,000 gallons (380,000 L) per day to the Warren Ohio POTW.

Zero-discharge CWTs do not discharge treated wastewater; instead, the wastewater is treated and reused in subsequent hydraulic fracturing operations. WVWRI (2012) state that this practice reduces potential effects on surface drinking water sources by reducing both direct and indirect discharges. Zero-discharge facilities may offer different levels of treatment including minimal treatment (for example, filtration), low-level treatment (chemical precipitation), and/or advanced treatment (evaporation, crystallization). Reserved Environmental Services (RES) Mt. Pleasant, Pennsylvania, is a zero liquid discharge facility permitted by PA DEP to treat wastewater from the Marcellus Shale play for reuse. Residual solids are dewatered and sent to a landfill. Treated wastewater effluent is stored, monitored, and chlorinated for reuse (ONG Services, 2015).

F.5. Water Quality for Reuse

As of 2015, there is no consensus on the water quality requirements for reuse of wastewater for hydraulic fracturing, and operator opinions vary on the minimum standards for the water quality needed for fracturing fluids (Vidic et al., 2013; Acharya et al., 2011). Table F-5 provides a list of constituents and the recommended or observed target concentrations for reuse applications. The wide concentration ranges for many constituents (e.g., TDS ranges from 500 to 70,000 mg/L), suggest that water quality requirements for reuse are dictated by operation-specific requirements, including operator preference and selection of fracturing fluid chemistry.

Table F-5. Water quality requirements for reuse.

Source: U.S. EPA (2015g).

Constituent	Reasons for Limiting Concentrations	Recommended or observed base fluid target concentrations (mg/L, after blending)[b]
TDS	Fluid stability	500 – 70,000
Chloride	Fluid stability	2,000 – 90,000
Sodium	Fluid stability	2,000 – 5,000
Metals		
Iron	Scaling	1 – 15
Strontium	Scaling	1
Barium	Scaling	2 – 38
Silica	Scaling	20
Calcium	Scaling	50 – 4,200
Magnesium	Scaling	10 – 1,000
Sulfate	Scaling	124 – 1,000
Potassium	Scaling	100 – 500
Scale formers[a]	Scaling	2,500

Constituent	Reasons for Limiting Concentrations	Recommended or observed base fluid target concentrations (mg/L, after blending)[b]
Other		
Phosphate	Not Reported	10
TSS	Plugging	50 – 1,500
Oil	Fluid stability	5 – 25
Boron	Fluid stability	0 – 10
pH (S.U.)	Fluid stability	6.5 – 8.1
Bacteria (counts/mL)	Bacterial growth	0 – 10,000

[a] Includes total of barium, calcium, manganese, and strontium.

[b] Unless otherwise noted.

Wastewater quality can be managed for reuse by either blending it with freshwater and allowing dilution to bring the concentrations of problematic constituents to an acceptable range or through treatment (Veil, 2010). Treatment, if needed, can be conducted at facilities that are mobile, semi-permanent modular systems, or fully permanent CWTs (Nicot et al., 2012). At a minimum, hydraulic fracturing service providers generally prefer that the wastewater be treated to remove TSS, microorganisms, and constituents that form scale or inhibit crosslinking in gelled fluid systems (Boschee, 2014). Figure F-8 shows a schematic of a treatment system to treat wastewater for reuse that can remove suspended solids, hardness, and organic constituents.

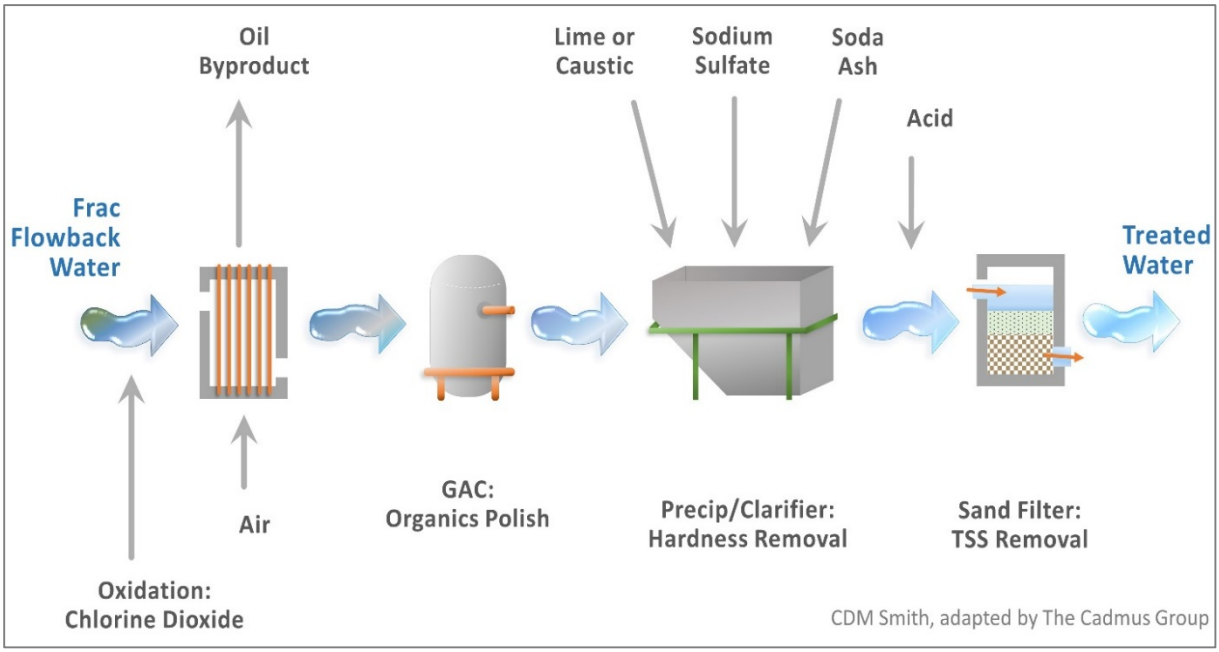

Figure F-8. Diagram of treatment for reuse of flowback and produced water.

Source: Kimball (2010).

In the Marcellus, the wastewater to be reused is first generally treated with oil/gas-water separation, filtration, and dilution (Ma et al., 2014). Although many Marcellus treatment facilities only supply basic reuse treatment that removes oil and solids, advanced treatment facilities that use techniques such as RO or distillation methods are also in operation (Veil, 2010).

Reuse concerns can vary with the type of hydraulic fracturing fluid used (e.g., slickwater, linear gel, crosslinked gel, foam) (Wasylishen and Fulton, 2012) and the anticipated changes in water chemistry over time (transition from flowback to produced water) (Hammer and VanBriesen, 2012). Elevated TDS is a concern, but residual constituents from previous fluid mixtures (e.g., breakers) may also cause difficulties when reusing water for subsequent fracturing operations (Montgomery, 2013; Walsh, 2013).

On-Site Treatment for Reuse

On-site systems that treat produced water for reuse can reduce potential impacts to drinking water resources associated with transportation and disposal and facilitate the logistics of reuse by preparing the water close to well sites. These systems sometimes consist of mobile units containing one or more treatment processes that can be moved from site to site to treat waters in newly developed sites that are not yet producing at full-scale. Semi-permanent facilities that serve a specific area also exist (Halldorson, 2013; Boschee, 2012).

Treatment systems are typically tailored for site-specific produced water chemical concentrations and desired water quality treatment goals, including whether significant TDS removal is needed. If

low TDS water is needed, more advanced treatment will be required (see Section 8.5 of Chapter 8), which can increase the treatment costs to three to four times higher than for treatment systems that do not remove TDS (Halldorson, 2013). On-site facilities may be warranted where truck hauling or seasonal accessibility to and from a central facility is an issue (Boschee, 2014; Tiemann et al., 2014). Operators may also consider on-site facilities if they have not fully committed to an area and the well counts are initially low. In those instances, they can later decide to add or remove units based on changing production volumes (Boschee, 2014).

F.6. Hydraulic Fracturing Impacts on POTWs

F.6.1. Potential Impacts on Treatment Processes

Wastewater treatment processes used by POTWs are generally not designed or operated for wastewater containing high salt concentrations (>0.1-5% salt). Four basic problems for biological treatment of saline water have been described (Woolard and Irvine, 1995): 1) microbes in conventional treatment systems tend to be sensitive to changes in ionic strength, 2) microbial metabolic functions are disrupted leading to decreased degradation of carbon compounds, 3) effluent suspended solids are increased due to cell lysis and/or a reduction in organisms that promote flocculation, and 4) the extent of salt acclimation is limited in conventional systems.

Biological pre-treatment may be beneficial as an added process in pre-treatment (e.g. prior to indirect discharge from a CWT to a POTW) for removal of organic contaminants. Specialized treatment systems using salt-tolerant bacteria may be beneficial as an additional level of treatment for pre-treating (or polishing) wastewaters in centralized treatment systems. (These processes differ from conventional biological processes in standard wastewater treatment, which are not suitable for large volumes of UOG wastewater.) In particular, membrane bioreactors (MBRs) have been examined for the treatment of oil and gas wastewater (Dao et al., 2013; Kose et al., 2012; Miller, 2011). MBRs provide advantages over conventional aeration basin processes as they can be implemented into existing treatment trains more easily and have a much smaller footprint than aeration basins.

Because sudden increases in chloride concentration, above 5-8 g/L, may cause problems for wastewater treatment (Ludzack and Noran, 1965). POTWs planning to accept indirect discharge in the future may find it valuable to restrict influent salt concentrations to a level that will not disturb existing biological treatment processes.

F.7. Hydraulic Fracturing and DBPs

F.7.1.1. Disinfection By-Products

This section provides background information on disinfection by-products (DBPs) and their formation to support the discussion in Section 8.6.1 of Chapter 8 regarding impacts on surface waters and downstream drinking water utilities due to elevated bromide and iodide in hydraulic fracturing wastewaters.

Regulated DBPs are a small subset of the full spectrum of DBPs that include other chlorinated and brominated DBPs as well as nitrogenous and iodated DBPs. Some of the emerging unregulated DBPs may be more toxic than their regulated counterparts (Harkness et al., 2015; McGuire et al., 2014; Parker et al., 2014). Of the many types of DBPs that can form when drinking water is disinfected, SDWA's Stage 1 and Stage 2 DBP Rules regulate four total trihalomethanes (TTHMs), five haloacetic acids (HAA5s), bromate, and chlorite (U.S. EPA, 2006).

Most brominated DBPs form when water containing organic material and bromide reacts with a disinfectant such as chlorine during drinking water treatment. Parameters that affect DBP formation include concentration and type of organic material, disinfectant concentration, pH, water temperature, and disinfectant contact time. In addition, many studies have found that elevated bromide levels correlate with increased DBP formation (Singer, 2010; Obolensky and Singer, 2008; Matamoros et al., 2007; Hua et al., 2006; Yang and Shang, 2004). Some studies found similar results for iodide as well (McGuire et al., 2014; Parker et al., 2014). Pope et al. (2007) reported that increased bromide levels are the second best indicator of DBP formation, with pH being the first.

In addition, research finds that higher levels of bromide and iodide contribute to increased concentrations of the brominated and iodated forms of DBPs (both regulated and unregulated), which tend to be more cytotoxic, genotoxic, and carcinogenic than chlorinated species (McGuire et al., 2014; Parker et al., 2014; States et al., 2013; Krasner, 2009; Richardson et al., 2007). Studies generally report that the ratios of halogen incorporation into DBPs reflect the ratio of halogen concentrations in the source water (Criquet et al., 2012; Jones et al., 2012; Obolensky and Singer, 2008).

From a regulatory perspective, elevated bromide levels create difficulties in meeting drinking water MCLs. When the TTHMs are predominately in the form of brominated DBPs, the higher molecular weight of bromide (79.9 g/mol) relative to chloride (35.5 g/mol) causes the overall mass of the TTHM sum to increase. This can lead to elevated concentrations of TTHM, in turn potentially leading to violations of the TTHM MCL for the drinking water utility (Francis et al., 2009).

High bromide levels are also cited as causing formation of nitrogenous DBP N-nitrosodimethylamine (NDMA) in water disinfected with chloramines (Luh and Mariñas, 2012). Although NDMA is not regulated by the EPA as of early 2015, it is listed as a priority toxic pollutant, and the EPA is planning to evaluate NDMA and other nitrosamines as candidates for regulation during the six-year review of the Microbial and Disinfection Byproducts (MDBP) rules (U.S. EPA, 2014a).

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Appendix G

Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

Appendix G. Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

Appendix G provides detail and supporting information on the oral reference values (RfVs) and oral slope factors (OSFs) that were identified in Chapter 9 of this assessment.[1] Section G.1 provides detail on the criteria used to select sources of RfVs and OSFs for chemicals used or detected in hydraulic fracturing processes, and lists all sources of RfVs and OSFs that were considered for this study. Section G.2 provides a glossary of the toxicity value terminology that is used by these various sources. Lastly, all of the RfVs and OSFs collected from these sources are provided in Table G-1 and Table G-2. Tables G-1a through G-1d show the available RfVs and OSFs for chemicals used in hydraulic fracturing fluids, and Tables G-2a through G-2d show the available RfVs and OSFs for chemicals detected in hydraulic fracturing flowback and wastewater. These tables provide cancer weight-of-evidence (WOE) characterizations for these chemicals where available, and indicate whether each chemical has available data on physicochemical properties or occurrence.

G.1. Criteria for Selection and Inclusion of Reference Value (RfV) and Oral Slope Factor (OSF) Data Sources

The criteria listed below were used to evaluate the quality of RfVs and OSFs considered for use in the hazard analyses conducted in Chapter 9. These criteria were originally outlined in the hydraulic fracturing research plan (U.S. EPA, 2011a) and interim progress report (U.S. EPA, 2012c). Only data sources that met these criteria were considered of sufficient quality to be included in the analyses.

The following criteria had to be met for a source to be deemed of sufficient quality:

1) The body or organization generating or producing the peer-reviewed RfVs, peer-reviewed OSFs, or peer reviewed qualitative assessment must be a governmental or intergovernmental body.
    a. Governmental bodies include sovereign states, and federated states/units.
    b. Intergovernmental bodies are those whose members are sovereign states, and the subdivisions or agencies of such intergovernmental bodies. The United Nations is an example of an intergovernmental body. The International Agency for Research on Cancer (IARC) is an agency of the World Health Organization (WHO), which is itself an agency of the United Nations. Thus, IARC is considered a subdivision of the United Nations.

[1] As defined in Chapter 9, the term RfV refers to reference values for noncancer effects occurring via the oral route of exposure and for chronic durations, except where noted.

2) The data source must include peer-reviewed RfVs, peer-reviewed OSFs, or peer reviewed qualitative assessments.
    a. A committee that is established to derive the RfVs, OSFs, or qualitative assessments can have members of that same committee provide the peer review, so long as either the entire committee, or members of the committee who did not participate in the derivation of a specific section of a work product, conduct the review.
    b. Peer reviewers who work for grantees of the organization deriving the RfVs, OSFs, or qualitative assessments are generally allowed, and this will not be considered to constitute a conflict/duality of interest.
    c. Peer reviewers may work in the same or different office, so long as they did not participate in any way in the development of the product, and these individuals must be free of conflicts/duality of interest with respect to the chemical(s) assigned.
        i. For instance, peer reviewers for Program X, conducted by Office A, may also be employed by Office A so long as they did not participate in the creation of the Program X product they are reviewing.

3) The RfVs, OSFs, or qualitative assessments must be based on peer-reviewed scientific data.
    a. There are cases where industry reports that were not published in a peer-reviewed, scholarly journal may be used, if the industry report has been adequately peer-reviewed by an external body (external to the group generating the report, and external to the group generating the peer-reviewed RfVs, peer-reviewed OSFs, or peer-reviewed qualitative assessment) that is free of conflicts/dualities of interest.

4) The RfVs, OSFs, or qualitative assessments must be focused on protection of the general public.
    a. Sources that are focused on workers are not appropriate as workers are assumed to accommodate additional risk than the general public due to their status as workers.

5) The body generating the values or qualitative assessments must be free of conflicts of interest with respect to the chemicals for which it derives RfVs, OSFs, or qualitative assessments.
    a. If a body generating the RfVs, OSFs, or qualitative assessments accepts funding from an interested party (i.e., a company or organization that may be impacted by past, present, or future values or qualitative assessments), then the body has a conflict of interest.
    b. For instance, if a non-profit organization is funded by an industry trade group, and the non-profit generates RfVs, OSFs, or qualitative assessments for chemicals that trade group is interested in, then the non-profit is considered to have a conflict of interest with respect to those chemicals.

It is important to note that having a conflict/duality of interest for one chemical is sufficient to disqualify the entire database, as it is assumed that conflicts/dualities of interest may exist for other chemicals as well.

G.1.1. Included Sources

We applied our criteria to 16 different sources of RfVs and/or OSFs. After application of our criteria, we were left with eight sources. For those sources which did not meet our criteria, we provide an explanation of why they were excluded.

The following sources were evaluated, met our criteria, and were selected as sources of reference doses or cancer slope factors for this analysis:

- **U.S. EPA Integrated Risk Information System (IRIS)**
- **U.S. EPA Human Health Benchmarks for Pesticides (HHBP)**
- **U.S. EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs)**
- **U.S. Agency for Toxic Substances and Disease Registry (ATSDR) Minimum Risk Levels (MRLs)**
- **California EPA Toxicity Criteria Database**
- **International Programme On Chemical Safety (IPCS) Concise International Chemical Assessment Documents (CICAD)**

The following sources were evaluated, met our criteria, and were selected as sources of qualitative cancer classifications:

- **International Agency for Research on Cancer (IARC)**
- **US National Toxicology Program Report on Carcinogens (RoC)**

RfVs and/or OSFs from these data sources are listed in Tables G-1a through G-1d for chemicals used in hydraulic fracturing fluid formulation, and Tables G-2a through G-2d for chemicals reported in hydraulic fracturing flowback and produced water.

In addition, Table G-1 and Table G-2 also list the EPA's drinking water maximum contaminant levels (MCLs) and maximum contaminant goal levels (MCLG) when available. These values are generally based on IRIS values, and are treatment-based. MCL and MCLG values are listed for reference only, and were not considered in the hazard analysis presented in Chapter 9.

G.1.2. Excluded Sources

- **American Conference of Governmental Industrial Hygienists:** The assessments derived by this body are specific to workers and are not generalizable to the general public. In addition, this body is not a governmental or intergovernmental body. Thus, these values were excluded based on criteria 1 and 4.
- **European Chemicals Bureau, Classification and Labeling Annex I of Directive 67/548/EEC:** These assessments are not based on peer-reviewed values, but are based on data supplied by manufacturers. Further, the enabling legislation states that "Manufacturers, importers, and downstream users shall examine the information…to ascertain whether it is adequate, reliable and scientifically valid for the purpose of the

evaluation…" This clearly demonstrates that the data and the evaluation are not required to be peer-reviewed. Thus, these values were excluded based on criterion 2.

- **Toxicology Excellence for Risk Assessment's (TERA's) International Toxicity Estimates for Risk Assessment (ITER):** The ITER database is developed by TERA a 501(c)(3) non-profit. TERA accepts funding from various sources, including interested parties that may be impacted by their assessment work. Thus, ITER is excluded based on criteria 1 and 5.
- **Other U.S. states:** The EPA evaluated values from all states that had values reported on their websites. If a state's values were determined to be largely duplicative of the EPA's values (e.g., the state adopts EPA values, such as the regional screening levels, and does not typically generate its own peer-reviewed values), that state's values were no longer considered. The EPA contacted those states whose values were determined to not be duplicative of EPA's values, and confirmed whether or not a peer review process was used to develop the state's values. The EPA determined that of the states with values not duplicative of the EPA's values, only California's values met all of the EPA's criteria for this report. Other states with publicly accessible RfVs and/or OSFs include: Alabama, Florida, Hawaii, and Texas.
- **WHO Guidelines for Drinking-Water Quality:** The WHO Guidelines' values are not RfVs, but rather drinking water values.

G.2. Glossary of Toxicity Value Terminology

This section defines the toxicity values and qualitative cancer classifications that are frequently found in the sources identified above.

Lowest-observed-adverse-effect level (LOAEL): The lowest exposure level at which there are biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group. Source: U.S. EPA (2011c).

Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level. Source: OEHHA (2012).

Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards. Source: U.S. EPA (2014b).

Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals. Source: U.S. EPA (2014b).

Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse),

noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects.

- **Chronic MRL:** Duration of exposure is 365 days or longer.
- **Intermediate MRL:** Duration of exposure is >14 to 364 days.
- **Acute MRL**: Duration of exposure is 1 to 14 days.

Source: ATSDR (2009).

No-observed-adverse-effect level (NOAEL): The highest exposure level at which there are no biologically significant increases in the frequency or severity of adverse effect between the exposed population and its appropriate control; some effects may be produced at this level, but they are not considered adverse or precursors of adverse effects. Source: U.S. EPA (2011c).

Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100. Source: U.S. EPA (2011c).

Reference dose (RfD) (U.S. EPA IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a NOAEL, LOAEL, or benchmark dose, with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments.

- **Chronic RfD:** Duration of exposure is up to a lifetime.
- **Subchronic RfD (sRFD)**: Duration of exposure is up to 10% of an average lifespan.

Source: U.S. EPA (2011c).

Reference dose (RfD) (U.S. EPA HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for IRIS and PPRTV RfD determination. Source: U.S. EPA (2015e).

Tolerable daily intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk. Source: WHO (2015).

Weight-of-evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans.

- **EPA 1986 guidelines:** Under the EPA's 1986 risk assessment guidelines, the WOE was described by categories "A through E," with Group A for known human carcinogens through Group E for agents with evidence of noncarcinogenicity. Five standard WOE descriptors were used:
    - A: Human carcinogen
    - B1: Probable human carcinogen—based on limited evidence of carcinogenicity in humans and sufficient evidence of carcinogenicity in animals
    - B2: Probable human carcinogen—based on sufficient evidence of carcinogenicity in animals
    - C: Possible human carcinogen
    - D: Not classifiable as to human carcinogenicity
    - E: Evidence of noncarcinogenicity for humans

  Source: U.S. EPA (2011c).

- **EPA 1996 proposed guidelines:** The EPA's 1996 proposed guidelines outlined a major change in the way hazard evidence was weighted in reaching conclusions about the human carcinogenic potential of agents. These guidelines replaced the WOE letter categories with the use of standard descriptors of conclusions incorporated into a brief narrative. Three categories of descriptors with the narrative were used:
    - Known/likely
    - Cannot be determined
    - Not likely

  Source: U.S. EPA (1996).

- **EPA 1999 guidelines:** The 1999 guidelines adopted a framework incorporating hazard identification, dose-response assessment, exposure assessment, and risk characterization with an emphasis on characterization of evidence and conclusions in each part of the assessment. Five descriptors summarizing the WOE in the narrative were used:
    - Carcinogenic to humans
    - Likely to be carcinogenic to humans
    - Suggestive evidence of carcinogenicity, but not sufficient to assess human carcinogenic potential
    - Data are inadequate for an assessment of human carcinogenic potential
    - Not likely to be carcinogenic to humans

  Source: U.S. EPA (1999).

- **EPA 2005 guidelines:** The approach outlined in the EPA's 2005 guidelines for carcinogen risk assessment considers all scientific information in determining whether and under what conditions an agent may cause cancer in humans and provides a narrative approach to

characterize carcinogenicity rather than categories. Five standard WOE descriptors are used as part of the narrative:

- Carcinogenic to humans
- Likely to be carcinogenic to humans
- Suggestive evidence of carcinogenic potential
- Inadequate information to assess carcinogenic potential
- Not likely to be carcinogenic to humans

Source: U.S. EPA (2011c).

- **IARC Monographs on the evaluation of carcinogenic risks to humans**: The IARC classifies carcinogen risk as a matter of scientific judgement that reflects the strength of the evidence derived from studies in humans, in experimental animals, from mechanistic data, and from other relevant data. Five WOE classifications are used:
  - Group 1: Carcinogenic to humans
  - Group 2A: Probably carcinogenic to humans
  - Group 2B: Possibly carcinogenic to humans
  - Group 3: Not classifiable as to its carcinogenicity to humans
  - Group 4: Probably not carcinogenic to humans

  Source: IARC (2015).
- **NTP:** The NTP describes the results of individual experiments on a chemical agent and notes the strength of the evidence for conclusions regarding each study. Negative results, in which the study animals do not have a greater incidence of neoplasia than control animals, do not necessarily mean that a chemical is not a carcinogen, inasmuch as the experiments are conducted under a limited set of conditions. Positive results demonstrate that a chemical is carcinogenic for laboratory animals under the conditions of the study and indicate that exposure to the chemical has the potential for hazard to humans. For each separate experiment, one of the following five categories is selected to describe the findings. These categories refer to the strength of the experimental evidence and not to potency or mechanism.
  - Clear evidence of carcinogenic activity
  - Some evidence of carcinogenic activity
  - Equivocal evidence of carcinogenic activity
  - No evidence of carcinogenic activity
  - Inadequate study of carcinogenic activity

  Source: NTP (2014a).
- **The RoC** is a congressionally mandated, science-based, public health report that identifies agents, substances, mixtures, or exposures (collectively called "substances") in our

environment that may potentially put people in the United States at increased risk for cancer. NTP prepares the RoC on behalf of the Secretary of the Health and Human Services. The listing criteria in the RoC Document are:

- Known to be a human carcinogen
- Reasonably anticipated to be a human carcinogen

Source: NTP (2014b).

G.3. Tables

Table G-1a. Chemicals reported to be used in hydraulic fracturing fluids, with available federal chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by IRIS reference dose (RfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

				IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
Chemical Name	**CASRN**	**Frac-Focus data available**	**Physico-chemical data available**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic oral MRL[d] (mg/kg-day)**	**Chronic RfD[e] (mg/kg-day)**	**Public health goal[f] (MCLG) (mg/L)**	**MCL[g] (mg/L)**
Acrylamide	79-06-1	x	x	0.002	0.5	"Likely to be carcinogenic to humans"	--	--	--	0.001	--	0	--
Propargyl alcohol	107-19-7	x	x	0.002	--	--	--	--	--	--	--	--	--
Furfural	98-01-1	x	x	0.003	--	--	--	--	--	--	0.01	--	--
Benzene	*71-43-2*	*x*	*x*	*0.004*	*0.015-0.055*	*A*	--	--	--	*0.0005*	--	*0*	*0.005*
Dichloromethane	*75-09-2*	*x*	*x*	*0.006*	*0.002*	*"Likely to be carcinogenic in humans"*	--	--	--	*0.06*	--	*0*	*0.005*
Naphthalene	*91-20-3*	*x*	*x*	*0.02*	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1,4-Dioxane	*123-91-1*	*x*	*x*	*0.03*	*0.1*	*"Likely to be carcinogenic to humans"*	--	--	--	*0.1*	--	--	--
Sodium chlorite	7758-19-2	x		0.03	--	*"Data are inadequate to assess human carcinogen-icity"*	--	--	--	--	--	1	0.8
Chlorine dioxide	10049-04-4	x		0.03	--	"Data are inadequate to assess human carcinogen-icity"	--	--	--	--	--	--	--
1,3-Dichloropropene	542-75-6	x	x	0.03	0.05	"Likely to be a human carcinogen"	--	--	--	0.03	--	--	--
Bisphenol A	80-05-7	x	x	0.05	--	--	--	--	--	--	--	--	--
Toluene	*108-88-3*	*x*	*x*	*0.08*	--	*"Inadequate information to assess the carcinogenic potential"*	--	--	--	--	--	*1*	*1*
Ethylbenzene	*100-41-4*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	*0.7*	*0.7*

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1-Butanol	71-36-3	x	x	0.1	--	D	--	--	--	--	--	--	--
Cumene	*98-82-8*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Acetophenone	*98-86-2*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
2-Butoxyethanol	111-76-2	x	x	0.1	--	"Not likely to be carcino-genic to humans"	--	--	--	--	--	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.2*	--	*"Data are inadequate to assess the carcinogenic potential"*	--	--	--	*0.2*	--	*10*	*10*
Formaldehyde	50-00-0	x	x	0.2	--	B1	--	--	--	0.2	--	--	--
Phenol	*108-95-2*	*x*	*x*	*0.3*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
2-Methyl-1-propanol	78-83-1	x	x	0.3	--	--	--	--	--	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Acetone	*67-64-1*	*x*	*x*	*0.9*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Ethyl acetate	141-78-6	x	x	0.9	--	--	--	--	IN	--	--	--	--
Ethylene glycol	*107-21-1*	*x*	*x*	*2*	--	--	--	--	--	--	--	--	--
Methanol	*67-56-1*	*x*	*x*	*2*	--	--	--	--	--	--	--	--	--
Benzoic acid	65-85-0	x	x	4	--	D	--	--	--	--	--	--	--
Aniline	62-53-3	x	x	--	0.0057	B2	0.007	--	--	--	--	--	--
Benzyl chloride	100-44-7	x	x	--	0.17	B2	0.002	--	--	--	--	--	--
(E)-Crotonaldehyde	123-73-9	x	x	--	--	C	0.001	--	--	--	--	--	--
N,N-Dimethylform amide	68-12-2	x	x	--	--	--	0.1	--	IN	--	--	--	--
Epichlorohydrin	106-89-8	x	x	--	0.0099	B2	0.006	--	--	--	--	0	--
1,2-Propylene glycol	*57-55-6*	*x*	*x*	--	--	--	*20*	--	*NL*	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
2-(2-Butoxyethoxy) ethanol	112-34-5	x	x	--	--	--	0.03	--	IN	--	--	--	--
Hexanedioic acid	124-04-9	x	x	--	--	--	2	--	--	--	--	--	--
Quinoline	91-22-5	x	x	--	3	”Likely to be carcinogenic in humans”	--	--	--	--	--	--	--
Ethylenediamine	107-15-3	x	x	--	--	D	0.09	--	IN	--	--	--	--
Formic acid	*64-18-6*	*x*	*x*	--	--	--	*0.9*	--	*IN*	--	--	--	--
Sodium chlorate	7775-09-9	x		--	--	--	--	--	--	--	0.03	--	--
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	x		--	--	--	--	--	--	--	0.44	--	--
Benzenesulfonic acid, C10-16-alkyl derivs.	68584-22-5	x		--	--	--	--	--	--	--	0.5	--	--
Ammonium phosphate	7722-76-1	x		--	--	--	49	--	IN	--	--	--	--
Didecyldimethylam monium chloride	7173-51-5	x	x	--	--	--	--	--	--	--	0.1	--	--
2-(Thiocyano methylthio)benzot hiazole	21564-17-0	x	x	--	--	--	--	--	--	--	0.01	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Mineral oil - includes paraffin oil	8012-95-1	x		--	--	--	3	--	IN	--	--	--	--
Trisodium phosphate	7601-54-9	x		--	--	--	49	--	IN	--	--	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		--	--	--	49	--	IN	--	--	--	--
Aluminum	*7429-90-5*	*x*		--	--	--	*1*	--	*IN*	*1*	--	--	--
Phosphoric acid	7664-38-2	x		--	--	--	48.6	--	IN	--	--	--	--
Iron	*7439-89-6*	*x*		--	--	--	*0.7*	--	*IN*	--	--	--	--
Tricalcium phosphate	7758-87-4	x		--	--	--	49	--	IN	--	--	--	--
Bis(2-chloroethyl) ether	*111-44-4*	*x*	*x*	--	*1.1*	*B2*	--	--	--	--	--	--	--
Dodecylbenzenesulfonic acid	27176-87-0	x	x	--	--	--	--	--	--	--	0.5	--	--
Hydrazine	302-01-2	x		--	3	B2	--	--	--	--	--	--	--
Tetrasodium pyrophosphate	7722-88-5	x		--	--	--	49	--	IN	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Potassium phosphate, tribasic	7778-53-2	x		--	--	--	49	--	IN	--	--	--	--
Sodium trimetaphosphate	7785-84-4	x		--	--	--	49	--	IN	--	--	--	--
Arsenic	*7440-38-2*			*0.0003*	*1.5*	*A*	--	--	--	*0.0003*	--	*0*	*0.010*
Phosphine	7803-51-2			0.0003	--	D	--	--	--	--	--	--	--
Acrolein	*107-02-8*		*x*	*0.0005*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Chromium (VI)	*18540-29-9*			*0.003*	--	*A (inhaled); D(oral)*	--	--	--	*0.0009*	--	--	--
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	*0.02*	*0.014*	*B2*	--	--	--	*0.06*	--	*0*	*0.006*
Chlorine	*7782-50-5*			*0.1*	--	--	--	--	--	--	--	--	--
Styrene	100-42-5		x	0.2	--	--	--	--	--	--	--	0.1	0.1

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Zinc	*7440-66-6*			*0.3*	--	*"Inadequate information to assess carcinogenic potential"*	--	--	--	*0.3*	--	--	--
Acrylic acid	79-10-7		x	0.5	--	--	--	--	IN	--	--	--	--
Chromium (III)	*16065-83-1*			*1.5*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Phthalic anhydride	85-44-9		x	2	--	--	--	--	--	--	--	--	--
Cyclohexanone	108-94-1		x	5	--	--	--	--	IN	--	--	--	--
1,2-Propylene oxide	75-56-9		x	--	0.24	B2	--	--	--	--	0.001	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	--	--	--	0.06	--	IN	--	--	--	--
Tributyl phosphate	126-73-8		x	--	--	--	0.01	0.009	LI	0.08	--	--	--
2-Methoxyethanol	109-86-4		x	--	--	--	0.005	--	IN	--	--	--	--
Polyphosphoric acids, sodium salts	68915-31-1			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, diammonium salt	7783-28-0			--	--	--	49	--	IN	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Sodium pyrophosphate	7758-16-9			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, aluminium sodium salt	7785-88-8			--	--	--	49	--	IN	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

[a] Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

[c] Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

[d] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

[e] Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

[f] Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

[g] Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

Table G-1b. Chemicals reported to be used in hydraulic fracturing fluids, with available state chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Ethylene oxide	75-21-8	x	x	20	0.31
Benzene	*71-43-2*	*x*	*x*	*24*	*0.1*
N-Methyl-2-pyrrolidone	872-50-4	x	x	17000	--
Acrylamide	79-06-1	x	x	140	4.5
Aniline	62-53-3	x	x	--	0.0057
Benzyl chloride	100-44-7	x	x	--	0.17
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*0.027*
Epichlorohydrin	106-89-8	x	x	--	0.08
Ethylbenzene	*100-41-4*	*x*	*x*	--	*0.011*
Nitrilotriacetic acid	139-13-9	x	x	--	0.0053
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	x	x	--	0.01
Thiourea	62-56-6	x	x	--	0.072
Bis(2-chloroethyl) ether	*111-44-4*	*x*	*x*	--	*2.5*
1,3-Butadiene	106-99-0	x	x	--	0.6
Hydrazine	302-01-2	x		--	3
1,3-Dichloropropene	542-75-6	x	x	--	0.091
Dichloromethane	*75-09-2*	*x*	*x*	--	*0.014*
Lead	*7439-92-1*			*0.5*	*0.0085*
Chromium (VI)	*18540-29-9*			*8.2*	*0.5*
2-Methoxyethanol	109-86-4		x	63	--
2-Ethoxyethanol	110-80-5		x	750	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	*20 (neonate male)* *58 (infant male)* *410 (adult)*	*0.003*
1,2-Propylene oxide	75-56-9		x	--	0.24
Arsenic	*7440-38-2*			--	*9.5*

[a] Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

Table G-1c. Chemicals reported to be used in hydraulic fracturing fluids, with available international chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by CICAD reference dose (TDI, or tolerable daily intake). An "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physicochemical data available	IPCS Chronic TDI[a] (mg/kg-day)
D-Limonene	5989-27-5	x	x	0.1
Potassium iodide	7681-11-0	x		0.01
Sodium iodide	7681-82-5	x		0.01
Copper(I) iodide	7681-65-4	x		0.01
Glyoxal	107-22-2	x	x	0.2
Ethylene glycol	*107-21-1*	*x*	*x*	*0.05*
N-Methyl-2-pyrrolidone	872-50-4	x	x	0.6
Strontium chloride	10476-85-4			0.13
Chromium (VI)	*18540-29-9*			*0.0009*

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

[a] Tolerable daily intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

Table G-1d. Chemicals reported to be used in hydraulic fracturing fluids, with available less-than-chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Benzyl chloride	100-44-7	x	x	0.002	--	--
Epichlorohydrin	106-89-8	x	x	0.006	--	--
(E)-Crotonaldehyde	123-73-9	x	x	0.01	--	--
Benzene	*71-43-2*	*x*	*x*	*0.01*	--	--
Ethylbenzene	*100-41-4*	*x*	*x*	*0.05*	--	*0.4*
Ethylenediamine	107-15-3	x	x	0.2	--	--
N,N-Dimethylformamide	68-12-2	x	x	0.3	--	--
2-(2-Butoxyethoxy)ethanol	112-34-5	x	x	0.3	--	--
Hexane	110-54-3	x	x	0.3	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.4*	*1*	*0.4*
Antimony trioxide	1309-64-4	x		0.5	--	--
Iron	*7439-89-6*	*x*		*0.7*	--	--
Toluene	*108-88-3*	*x*	*x*	*0.8*	*0.8*	*0.02*
Formic acid	*64-18-6*	*x*	*x*	*0.9*	--	--
Hexanedioic acid	124-04-9	x	x	2	--	--
Benzoic acid	65-85-0	x	x	4	--	--
1,2-Propylene glycol	*57-55-6*	*x*	*x*	*20*	--	--
Mineral oil - includes paraffin oil	8012-95-1	x		30	--	--
Phosphoric acid	7664-38-2	x		48.6	--	--
Ammonium phosphate	7722-76-1	x		49	--	--
Trisodium phosphate	7601-54-9	x		49	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		49	--	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Tricalcium phosphate	7758-87-4	x		49	--	--
Tetrasodium pyrophosphate	7722-88-5	x		49	--	--
Potassium phosphate, tribasic	7778-53-2	x		49	--	--
Sodium trimetaphosphate	7785-84-4	x		49	--	--
Acrylamide	79-06-1	x	x	--	0.01	0.001
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*5*	*0.5*
Ethylene glycol	*107-21-1*	*x*	*x*	--	*0.8*	*0.8*
Naphthalene	*91-20-3*	*x*	*x*	--	*0.6*	*0.6*
Phenol	*108-95-2*	*x*	*x*	--	*1*	--
Sodium chlorite	7758-19-2	x		--	--	0.1
Acetone	*67-64-1*	*x*	*x*	--	--	*2*
2-Butoxyethanol	111-76-2	x	x	--	0.4	0.07
Aluminum	*7429-90-5*	*x*		--	--	*1*
Formaldehyde	50-00-0	x	x	--	--	0.3
1,3-Dichloropropene	542-75-6	x	x	--	--	0.04
Dichloromethane	*75-09-2*	*x*	*x*	--	*0.2*	--
Antimony trichloride	10025-91-9			0.0004	--	--
2-Methoxyethanol	109-86-4		x	0.02	--	--
Tributyl phosphate	126-73-8		x	0.03	1.1	0.08
Acrylic acid	79-10-7		x	0.2	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	0.6	--	--
Cyclohexanone	108-94-1		x	2	--	--
Polyphosphoric acids, sodium salts	68915-31-1			49	--	--
Phosphoric acid, diammonium salt	7783-28-0			49	--	--
Sodium pyrophosphate	7758-16-9			49	--	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Phosphoric acid, aluminium sodium salt	7785-88-8			49	--	--
Acrolein	*107-02-8*		*x*	--	--	*0.004*
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	--	--	*0.1*
Styrene	100-42-5		x	--	0.1	--
Arsenic	*7440-38-2*			--	*0.005*	--
Chromium (VI)	*18540-29-9*			--	--	*0.005*
Copper	*7440-50-8*			--	*0.01*	*0.01*
Zinc	*7440-66-6*			--	--	*0.3*

[a] Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRFD): Duration of exposure is up to 10% of an average lifespan.

[b] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

[c] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

Table G-2a. Chemicals reported to be detected in flowback or produced water, with available federal chronic RfVs and OSFs.

Chemicals are ranked by IRIS reference dose (RfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

				IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
Chemical Name	**CASRN**	**Concen-tration data available**	**Physico-chemical data available**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic oral MRL[d] (mg/kg-day)**	**Chronic RfD[e] (mg/kg-day)**	**Public health goal[f] (MCLG) (mg/L)**	**MCL[g] (mg/L)**
Heptachlor epoxide	1024-57-3		x	0.000013	9.1	B2	--	--	--	--	--	0	0.0002
Phosphorus	7723-14-0	x		0.00002	--	D	--	--	--	--	--	--	--
Aldrin	309-00-2		x	0.00003	17	B2	--	--	--	0.00003	--	--	--
Dieldrin	60-57-1		x	0.00005	16	B2	--	--	--	0.00005	--	--	--
Arsenic	*7440-38-2*	x		*0.0003*	*1.5*	*A*	--	--	--	*0.0003*	--	*0*	*0.010*
Lindane	58-89-9		x	0.0003	--	--	--	--	--	--	--	0.0002	0.0002
Antimony	7440-36-0	x		0.0004	--	--	--	--	IN	--	--	0.006	0.006
Acrolein	*107-02-8*		*x*	*0.0005*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Cadmium	7440-43-9	x		0.0005 (water)	--	B1	--	--	--	0.0001	--	0.005	0.005
Heptachlor	76-44-8		x	0.0005	4.5	B2	--	--	--	--	--	0	0.0004

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Cyanide	57-12-5		x	0.0006	--	"Inadequate information to assess the carcinogenic potential"	--	--	--	--	--	0.2	0.2
Pyridine	110-86-1	x	x	0.001	--	--	--	--	--	--	--	--	--
Methyl bromide	74-83-9		x	0.0014	--	D	--	--	--	--	0.02	--	--
Beryllium	7440-41-7	x		0.002	--	B1	--	--	--	0.002	--	0.004	0.004
Chromium (VI)	*18540-29-9*			*0.003*	--	*A (inhaled); D(oral)*	--	--	--	*0.0009*	--	--	--
Benzene	*71-43-2*	*x*	*x*	*0.004*	*0.015-0.055*	*A*	--	--	--	*0.0005*	--	*0*	*0.005*
2-Methylnaphthalene	91-57-6	x	x	0.004	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	0.04	--	--	--
Molybdenum	7439-98-7	x		0.005	--	--	--	--	--	--	--	--	--
Silver	7440-22-4	x		0.005	--	D	--	--	--	--	--	--	--
Selenium	7782-49-2	x		0.005	--	D	--	--	--	0.005	--	0.05	0.05
Dichloromethane	*75-09-2*		*x*	*0.006*	*0.002*	*"Likely to be carcinogenic in humans"*	--	--	--	*0.06*	--	*0*	*0.005*

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1,2,4-Trichlorobenzene	120-82-1		x	0.01	--	D	--	0.029	LI	0.1	--	0.07	0.07
Tetrachloroethylene	127-18-4		x	0.006	0.0021	"Likely to be carcinogenic in humans"	--	--	--	0.008	--	0	0.005
Chloroform	67-66-3	x	x	0.01	--	B2	--	--	--	0.01	--	--	--
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	*0.02*	*0.014*	*B2*	--	--	--	*0.06*	--	*0*	*0.006*
Naphthalene	*91-20-3*	*x*	*x*	*0.02*	--	*"Data are inadequate to assess human carcinogenic potential"*	--	--	--	--	--	--	--
2,4-Dimethylphenol	105-67-9	x	x	0.02	--	--	--	--	IN	--	--	--	--
Chlorodibromomethane	124-48-1		x	0.02	0.084	C	--	--	--	0.09	--	--	--
Bromoform	75-25-2		x	0.02	0.0079	B2	--	--	--	0.02	--	--	--
Bromodichloromethane	75-27-4		x	0.02	0.062	B2	--	--	--	0.02	--	--	--
Diphenylamine	122-39-4	x	x	0.025	--	--	--	--	IN	--	0.1	--	--
1,4-Dioxane	*123-91-1*	*x*	*x*	*0.03*	*0.1*	*"Likely to be carcinogenic to humans"*	--	--	--	*0.1*	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Pyrene	129-00-0	x	x	0.03	--	D	--	--	--	--	--	--	--
Fluoranthene	206-44-0	x	x	0.04	--	D	--	--	IN	--	--	--	--
Fluorene	86-73-7	x	x	0.04	--	D	--	--	--	--	--	--	--
m-Cresol	108-39-4	x	x	0.05	--	C	--	--	--	--	--	--	--
o-Cresol	95-48-7	x	x	0.05	--	C	--	--	IN	--	--	--	--
Toluene	*108-88-3*	*x*	*x*	*0.08*	--	*"Inadequate information to assess the carcinogenic potential"*	--	--	--	--	--	*1*	*1*
Chlorine	*7782-50-5*			*0.1*	--	--	--	--	--	--	--	--	--
Ethylbenzene	*100-41-4*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	*0.7*	*0.7*
Cumene	*98-82-8*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Acetophenone	*98-86-2*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Carbon disulfide	75-15-0	x	x	0.1	--	--	--	--	--	--	--	--	--
Dibutyl phthalate	84-74-2	x	x	0.1	--	D	--	--	--	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Nitrite	14797-65-0	x		0.1	--	--	--	--	--	--	--	1	1
Manganese	7439-96-5	x		0.14	--	D	--	--	--	--	--	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.2*	--	*"Data are inadequate to assess the carcinogenic potential"*	--	--	--	*0.2*	--	*10*	*10*
Barium	7440-39-3	x		0.2	--	"Not likely to be carcinogenic to humans"	--	--	--	0.2	--	2	2
Boron	7440-42-8	x		0.2	--	"Data are inadequate to assess the carcinogenic potential"	--	--	--	--	--	--	--
Zinc	*7440-66-6*	x		*0.3*	--	*"Inadequate information to assess carcinogenic potential"*	--	--	--	*0.3*	--	--	--
Phenol	*108-95-2*	*x*	*x*	*0.3*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Strontium	7440-24-6	x		0.6	--	--	--	--	--	--	--	--	--
Methyl ethyl ketone	78-93-3		x	0.6	--	"Data are inadequate to assess carcinogenic potential"	--	--	--	--	--	--	--
Diethyl phthalate	84-66-2		x	0.8	--	D	--	--	--	--	--	--	--
Acetone	*67-64-1*	*x*	*x*	*0.9*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--
Chromium (III)	*16065-83-1*			*1.5*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--
Nitrate	14797-55-8	x		1.6	--	--	--	--	--	--	--	10	10
Ethylene glycol	*107-21-1*		*x*	*2*	--	--	--	--	--	--	--	--	--
Methanol	*67-56-1*		*x*	*2*	--	--	--	--	--	--	--	--	--
1,2-Propylene glycol	*57-55-6*		*x*	--	--	--	*20*	--	*NL*	--	--	--	--
Formic acid	*64-18-6*		*x*	--	--	--	*0.9*	--	*IN*	--	--	--	--
Aluminum	*7429-90-5*	*x*		--	--	--	*1*	--	*IN*	*1*	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Iron	*7439-89-6*	x		--	--	--	*0.7*	--	*IN*	--	--	--	--
Bis(2-chloroethyl) ether	*111-44-4*		*x*	--	*1.1*	*B2*	--	--	--	--	--	--	--
Benzyl alcohol	100-51-6	x	x	--	--	--	0.1	--	IN	--	--	--	--
Butylbenzene	104-51-8		x	--	--	--	0.05	--	IN	--	--	--	--
Acrylonitrile	107-13-1		x	--	0.54	B1	--	--	--	0.04	--	--	--
Phorate	298-02-2		x	--	--	--	--	--	--	--	0.0005	--	--
beta-Hexachloro cyclohexane	319-85-7		x	--	1.8	C	--	--	--	--	--	--	--
Benzo(a)pyrene	50-32-8	x	x	--	7.3	B2	--	--	--	--	--	0	0.0002
p,p'-DDE	72-55-9		x	--	0.34	B2	--	--	--	--	--	--	--
Lithium	7439-93-2	x		--	--	--	0.002	--	IN	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Cobalt	7440-48-4	x		--	--	--	0.0003	--	LI	--	--	--	--
Vanadium	7440-62-2	x		--	--	--	0.00007	--	IN	--	--	--	--
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.0049	B2	--	--	--	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

[a] Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

[c] Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

[d] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

[e] Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

[f] Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

[g] Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

Table G-2b. Chemicals reported to be detected in flowback or produced water, with available state chronic RfVs and OSFs.

Chemicals are ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Lead	*7439-92-1*	*x*		*0.5*	*0.0085*
Cadmium	7440-43-9	x		4.1	15
Chromium (VI)	*18540-29-9*			*8.2*	*0.5*
Dibutyl phthalate	84-74-2	x	x	8.7	--
Benzene	*71-43-2*	*x*	*x*	*24*	*0.1*
Acrylonitrile	107-13-1		x	--	1
1,4-Dioxane	*123-91-1*	*x*	*x*	*--*	*0.027*
Ethylbenzene	*100-41-4*	*x*	*x*	*--*	*0.011*
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	*20 (neonate male) 58 (infant male) 410 (adult)*	*0.003*
Arsenic	*7440-38-2*	*x*		*--*	*9.5*
Bis(2-chloroethyl) ether	*111-44-4*		*x*	*--*	*2.5*
Heptachlor epoxide	1024-57-3		x	--	5.5
1,2,4-Trichlorobenzene	120-82-1		x	--	0.0036
Tetrachloroethylene	127-18-4		x	--	0.051
Indeno(1,2,3-cd)pyrene	193-39-5	x	x	--	1.2
Benzo(b)fluoranthene	205-99-2	x	x	--	1.2
Benzo(k)fluoranthene	207-08-9	x	x	--	1.2
Aldrin	309-00-2		x	--	17
beta-Hexachlorocyclohexane	319-85-7		x	--	1.5
Benzo(a)pyrene	50-32-8	x	x	--	2.9
Dibenz(a,h)anthracene	53-70-3	x	x	--	4.1
7,12-Dimethylbenz(a)anthracene	57-97-6		x	--	250
Lindane	58-89-9		x	--	1.1
Dieldrin	60-57-1		x	--	16
Chloroform	67-66-3	x	x	--	0.019

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
p,p'-DDE	72-55-9		x	--	0.34
Bromoform	75-25-2		x	--	0.011
Bromodichloromethane	75-27-4		x	--	0.13
Heptachlor	76-44-8		x	--	4.1
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.009
Safrole	94-59-7		x	--	0.22
Dichloromethane	*75-09-2*		*x*	--	*0.014*

[a] Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

Table G-2c. Chemicals reported to be detected in flowback or produced water, with available international chronic RfVs and OSFs.

Chemicals are ranked by CICAD reference dose (TDI – Tolerable Daily Intake). An "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physicochemical data available	IPCS Chronic TDI[a] (mg/kg-day)
Heptachlor	76-44-8		x	0.0001
Strontium	7440-24-6	x		0.13
Chloroform	67-66-3	x	x	0.015
Mercury	7439-97-6	x		0.002
Barium	7440-39-3	x		0.02
Beryllium	7440-41-7	x		0.002
Ethylene glycol	*107-21-1*		*x*	*0.05*
Tetrachloroethene	127-18-4		x	0.05
Chromium (VI)	*18540-29-9*			*0.0009*
Diethyl phthalate	84-66-2		x	5

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

[a] Tolerable Daily Intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

Table G-2d. Chemicals reported to be detected in flowback or produced water, with available less-than-chronic RfVs and OSFs.

Chemicals are ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Aldrin	309-00-2		x	0.00004	0.002	--
Antimony	7440-36-0	x		0.0004	--	--
Vanadium	7440-62-2	x		0.0007	--	0.01
Lithium	7439-93-2	x		0.002	--	--
Cobalt	7440-48-4	x		0.003	--	0.01
2-Methylnaphthalene	91-57-6	x	x	0.004	--	--
Methyl bromide	74-83-9		x	0.005	--	0.003
Bromodichloromethane	75-27-4		x	0.008	0.04	--
1,2,3-Trichlorobenzene	87-61-6		x	0.008	--	--
Benzene	*71-43-2*	*x*	*x*	*0.01*	--	--
p-Cresol	106-44-5	x	x	0.02	--	--
Bromoform	75-25-2		x	0.03	0.7	0.2
Ethylbenzene	*100-41-4*	*x*	*x*	*0.05*	--	*0.4*
2,4-Dimethylphenol	105-67-9	x	x	0.05	--	--
Chlorodibromomethane	124-48-1		x	0.07	0.1	--
1,2,4-Trichlorobenzene	120-82-1		x	0.09	--	0.1
Butylbenzene	104-51-8		x	0.1	--	--
Benzyl alcohol	100-51-6	x	x	0.3	--	--
Pyrene	129-00-0	x	x	0.3	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.4*	*1*	*0.4*
Iron	*7439-89-6*	*x*		*0.7*	--	--
Toluene	*108-88-3*	*x*	*x*	*0.8*	*0.8*	*0.02*
Formic acid	*64-18-6*		*x*	*0.9*	--	--
1,2-Propylene glycol	*57-55-6*		*x*	*20*	--	--

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Acrolein	*107-02-8*		*x*	--	--	*0.004*
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*5*	*0.5*
Ethylene glycol	*107-21-1*		*x*	--	*0.8*	*0.8*
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	--	--	*0.1*
Naphthalene	*91-20-3*	*x*	*x*	--	*0.6*	*0.6*
Phenol	*108-95-2*	*x*	*x*	--	*1*	--
Acetone	*67-64-1*	*x*	*x*	--	--	*2*
Arsenic	*7440-38-2*	*x*		--	*0.005*	--
Chromium (VI)	*18540-29-9*			--	--	*0.005*
Copper	*7440-50-8*	*x*		--	*0.01*	*0.01*
Zinc	*7440-66-6*	*x*		--	--	*0.3*
Aluminum	*7429-90-5*	*x*		--	--	*1*
Acrylonitrile	107-13-1		x	--	0.1	0.01
Dioctyl phthalate	117-84-0	x	x	--	3	0.4
Tetrachloroethylene	127-18-4		x	--	0.008	0.008
Fluoranthene	206-44-0	x	x	0.1	--	0.4
beta-Hexachlorocyclohexane	319-85-7		x	--	0.05	0.0006
Lindane	58-89-9		x	--	0.003	0.00001
Dieldrin	60-57-1		x	--	--	0.0001
Chloroform	67-66-3	x	x	--	0.3	0.1
Strontium	7440-24-6	x		--	--	2
Tin	7440-31-5	x		--	--	0.3
Barium	7440-39-3	x		--	--	0.2
Boron	7440-42-8	x		--	0.2	0.2
Cadmium	7440-43-9	x		--	--	0.0005
Carbon disulfide	75-15-0	x	x	--	0.01	--
Heptachlor	76-44-8		x	--	0.0006	0.0001
Phosphorus	7723-14-0	x		--	--	0.0002

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Diethyl phthalate	84-66-2		x	--	7	6
Dibutyl phthalate	84-74-2	x	x	--	0.5	--
Fluorene	86-73-7	x	x	--	--	0.4
Dichloromethane	*75-09-2*		*x*	--	*0.2*	--

[a] Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRFD): Duration of exposure is up to 10% of an average lifespan.

[b] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

[c] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

G.4. References for Appendix G

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Appendix H

Description of EPA Hydraulic Fracturing Study Publications Cited in This Assessment

Appendix H. Description of EPA Hydraulic Fracturing Study Publications Cited in This Assessment

Table H-1. Titles, descriptions, and citations for EPA hydraulic fracturing study publications cited in this assessment.

Research project	Description	Citations
Analysis of existing data		
Literature Review	Review and assessment of existing papers and reports, focusing on peer-reviewed literature	Literature review is incorporated into this document.
Spills Database Analysis	Characterization of hydraulic fracturing-related spills using information obtained from selected state and industry data sources	U.S. EPA (U.S. Environmental Protection Agency). (2015). Review of state and industry spill data: characterization of hydraulic fracturing-related spills [EPA Report]. (EPA/601/R-14/001). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency.
Service Company Analysis	Analysis of information provided by nine hydraulic fracturing service companies in response to a September 2010 information request on hydraulic fracturing operations	Analysis of data received is incorporated into this document.[1]
Well File Review	Analysis of information provided by nine oil and gas operators in response to an August 2011 information request for 350 well files	U.S. EPA (U.S. Environmental Protection Agency). (2015). Review of well operator files for hydraulically fractured oil and gas production wells: Well design and construction [EPA Report]. (EPA/601/R-14/002). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency. Analysis of data received is also incorporated into this document.[2]

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Research project	Description	Citations
FracFocus Analysis	Analysis of data compiled from FracFocus 1.0, the national hydraulic fracturing chemical registry operated by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission	U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0 [EPA Report]. (EPA/601/R-14/003). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency. http://www2.epa.gov/hfstudy/analysis-hydraulic-fracturing-fluid-data-fracfocus-chemical-disclosure-registry-1-pdf U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0: project database. Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development. U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0: Data management and quality assessment report [EPA Report]. (EPA/601/R-14/006). Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development. http://www2.epa.gov/sites/production/files/2015-03/documents/fracfocus_data_management_report_final_032015_508.pdf

Research project	Description	Citations
Scenario evaluations		
Subsurface Migration Modeling	Numerical modeling of subsurface fluid migration scenarios that explore the potential for fluids, including liquids and gases to move from the fractured zone to drinking water aquifers	Kim, J; Moridis, GJ. (2013). Development of the T+M coupled flow–geomechanical simulator to describe fracture propagation and coupled flow–thermal–geomechanical processes in tight/shale gas systems. Computers and Geosciences 60: 184-198. http://dx.doi.org/10.1016/j.cageo.2013.04.023 Kim, J; Moridis, GJ. (In Press). Numerical analysis of fracture propagation during hydraulic fracturing operations in shale gas systems. International Journal of Rock Mechanics and Mining Sciences. Kim, J; Um, ES; Moridis, GJ. (2014). Fracture Propagation, Fluid Flow, and Geomechanics of Water-Based Hydraulic Fracturing in Shale Gas Systems and Electromagnetic Geophysical Monitoring of Fluid Migration. SPE Hydraulic Fracturing Technology Conference, The Woodlands, Texas, USA. http://dx.doi.org/10.2118/168578-MS Reagan, MT; Moridis, GJ; Johnson, JN; Keen, ND. (2015). Numerical simulation of the environmental impact of hydraulic fracturing of tight/shale gas reservoirs on near-surface groundwater: background, base cases, shallow reservoirs, short-term gas and water transport. Water Resour Res 51: 1-31. http://dx.doi.org/10.1002/2014WR016086 Rutqvist, J; Rinaldi, AP; Cappa, F; Moridis, GJ. (2013). Modeling of fault reactivation and induced seismicity during hydraulic fracturing of shale-gas reservoirs. Journal of Petroleum Science and Engineering 107: 31-44. http://dx.doi.org/10.1016/j.petrol.2013.04.023 Rutqvist, J; Rinaldi, AP; Cappa, F; Moridis, GJ. (2015). Modeling of fault activation and seismicity by injection directly into a fault zone associated with hydraulic fracturing of shale-gas reservoirs. Journal of Petroleum Science and Engineering 127: 377-386. http://dx.doi.org/10.1016/j.petrol.2015.01.019
Surface Water Modeling	Modeling of concentrations of selected chemicals at public water supplies downstream from wastewater treatment facilities that discharge treated hydraulic fracturing wastewater to surface waters	Weaver, JW; Xu, J; Mravik, SC. (In Press) Scenario analysis of the impact on drinking water intakes from bromide in the discharge of treated oil and gas waste water. J Environ Eng.

Research project	Description	Citations
Water Availability Modeling	Assessment and modeling of current and future scenarios exploring the impact of water usage for hydraulic fracturing on drinking water availability in the Upper Colorado River Basin and the Susquehanna River Basin	U.S. EPA (U.S. Environmental Protection Agency). (2015). Case study analysis of the impacts of water acquisition for hydraulic fracturing on local water availability [EPA Report]. (EPA/600/R-14/179). Washington, D.C.
Laboratory studies		
Source Apportionment Studies	Identification and quantification of the source(s) of high bromide and chloride concentrations at public water supply intakes downstream from wastewater treatment plants discharging treated hydraulic fracturing wastewater to surface waters	U.S. EPA (U.S. Environmental Protection Agency). (2015). Sources contributing bromide and inorganic species to drinking water intakes on the Allegheny river in western Pennsylvania [EPA Report]. (EPA/600/R-14/430). Washington, D.C.
Analytical Method Development	Development of analytical methods for selected chemicals found in hydraulic fracturing fluids or wastewater	DeArmond, PD; DiGoregorio, AL. (2013). Characterization of liquid chromatography-tandem mass spectrometry method for the determination of acrylamide in complex environmental samples. Anal Bioanal Chem 405: 4159-4166. http://dx.doi.org/10.1007/s00216-013-6822-4 DeArmond, PD; DiGoregorio, AL. (2013). Rapid liquid chromatography-tandem mass spectrometry-based method for the analysis of alcohol ethoxylates and alkylphenol ethoxylates in environmental samples. J Chromatogr A 1305: 154-163. http://dx.doi.org/10.1016/j.chroma.2013.07.017

Research project	Description	Citations
Analytical Method Development (cont.)	Development of analytical methods for selected chemicals found in hydraulic fracturing fluids or wastewater (cont.)	U.S. EPA (U.S. Environmental Protection Agency). (2014). Development of rapid radiochemical method for gross alpha and gross beta activity concentration in flowback and produced waters from hydraulic fracturing operations [EPA Report]. (EPA/600/R-14/107). Washington, D.C. http://www2.epa.gov/hfstudy/development-rapid-radiochemical-method-gross-alpha-and-gross-beta-activity-concentration U.S. EPA (U.S. Environmental Protection Agency). (2014). The verification of a method for detecting and quantifying diethylene glycol, triethylene glycol, tetraethylene glycol, 2-butoxyethanol and 2-methoxyethanol in ground and surface waters [EPA Report]. (EPA/600/R-14/008). Washington, D.C. http://www2.epa.gov/hfstudy/verification-method-detecting-and-quantifying-diethylene-glycol-triethylene-glycol
Retrospective case studies *Investigations of whether reported drinking water impacts may be associated with or caused by hydraulic fracturing activities*		
Las Animas and Huerfano Counties, Colorado	Investigation of potential drinking water impacts from coalbed methane extraction in the Raton Basin	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in the Raton Basin, Colorado: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/091). Washington, D.C.
Dunn County, North Dakota	Investigation of potential drinking water impacts from a well blowout during hydraulic fracturing for oil in the Bakken Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in Killdeer, North Dakota: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/103). Washington, D.C.
Bradford County, Pennsylvania	Investigation of potential drinking water impacts from shale gas development in the Marcellus Shale	U.S. EPA (U.S. Environmental Protection Agency). (2014). Retrospective case study in northeastern Pennsylvania: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/088). Washington, D.C.
Washington County, Pennsylvania	Investigation of potential drinking water impacts from shale gas development in the Marcellus Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in southwestern Pennsylvania: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/084). Washington, D.C.

Research project	Description	Citations
Wise County, Texas	Investigation of potential drinking water impacts from shale gas development in the Barnett Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in Wise County, Texas: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/090). Washington, D.C.

Appendix I

Unit Conversions

Appendix I. Unit Conversions

LENGTH

1 in (inch)	=	2.54 cm (centimeters)
		25.4 mm (millimeters)
		25,400 µm (microns)
1 ft (foot)	=	0.3048 m (meters)
		30.48 cm
1 mi (mile)	=	5,280 ft
		1,609.344 m
		1.6093 km (kilometers)

AREA

1 ft^2 (square foot)	=	0.0929 m^2 (square meters)
1 acre	=	43,560 ft^2
	=	0.0016 mi^2 (square miles)
	=	0.4047 ha (hectares)
	=	4,046.825 m^2
1 mi^2	=	639.9974 ac
	=	258.9988 ha
	=	2.5899 km^2 (square kilometers)

MASS

1 lb (pound)	=	453.5924 g (grams)
	=	0.4536 kg (kilograms)
1 ton (short ton, U.S.)	=	2,000 lbs
	=	907.185 kg
	=	0.9072 metric tons

VOLUME OR CAPACITY (LIQUID MEASURE)

1 bbl (barrel)	=	42 gal (gallons, U.S.)
	=	158.9873 L (liters)
1 gal	=	231 in^3 (cubic inches)
	=	0.1337 ft^3 (cubic feet)
	=	3.7854 L
	=	0.0039 m^3 (cubic meters)
	=	3.7854×10^{-9} Mm^3 (million cubic meters)
1 Mgal (million gallons)	=	1.3368×10^5 ft^3
1 ft^3	=	1,728 in^3
	=	7.4805 gal
	=	28.3169 L
	=	0.0283 m^3
1 mi^3 (cubic mile)	=	4.1682 km^3 (cubic kilometers)

CONCENTRATION

1 mg/L (milligram per liter)	=	1.0×10^{-6} kg/L (kilograms per liter)
	=	1.0×10^{-3} g/L (grams per liter)
	=	1,000 µg/L (micrograms per liter)
	=	1.001 ppm (parts per million)
	=	8.3454×10^{-6} lb/gal (pounds per gallon)
	=	6.2428×10^{-5} lb/ft^3 (pounds per cubic foot)

SPEED

1 mi/hr (mile per hour)	=	$1.466\overline{6}$ ft/s (feet per second)
	=	0.4470 m/s (meters per second)

DENSITY

1 g/mL	=	1,000 g/L
	=	1.0×10^6 mg/L

VOLUME PER UNIT TIME

1 ft^3/s (cubic foot per second)	=	448.8312 gpm (gallons per minute)
	=	0.6163 Mgpd (million gallons per day)
	=	28.3169 L/s (liters per second)
	=	0.0283 m^3/s (cubic meters per second)
1 ft^3/day (cubic feet per day)	=	0.0052 gpm
	=	7.4805 gpd
	=	0.0283 m^3/d (cubic meters per day)
1 bbl/day (barrel per day)	=	42 gpd
	=	158.9873 L/d (liters per day)

PRESSURE

1 psi (pound per square inch)	=	6,894.7573 Pa (pascals)
	=	0.068 atm (standard atmospheres)

RADIATION

Activity

1 Ci (curie)	=	3.7×10^{10} decays per second
1 Bq (becquerel)	≈	2.703×10^{-11} Ci
	≈	27.027 pCi (picocuries)
1 pCi	=	0.037 Bq
	=	0.037 decays per second
	=	2.22 decays per minute

Exposure

1 rem (röentgen equivalent in man)	=	0.01 Sv (sieverts)
1 Sv	=	1 J/kg (joule per kilogram)

ELECTRIC CONDUCTANCE

1 S (siemen)	=	1 Ω^{-1} (reciprocal of resistance)
	=	1 A/V (ampere per volt)
	=	1 $kg^{-1} \bullet m^{-2} \bullet s^3 \bullet A^2$ (second cubed- ampere squared per kilogram-square meter)
	=	1.0×10^6 μS (microsiemens)

TEMPERATURE

[°F (degrees, Fahrenheit) - 32] × 5/9 = °C (degrees, Celsius)

PERMEABILITY

1 cm^2	=	1.0×10^{-4} m^2
	≈	1.0×10^{8} D (darcys)
1 D	≈	1.0×10^{-12} m^2
	=	1,000 mD (millidarcys)
	=	1.0×10^{6} μD (microdarcys)

Appendix J

Glossary

Appendix J. Glossary

J.1. Glossary Terms and Definitions

Acid mine drainage: Flow of water from areas that have been mined for coal or other mineral ores. The water has a low pH because of its contact with sulfur-bearing material and is harmful to aquatic organisms. (U.S. EPA, 2013d)

Additive: A single chemical or chemical mixture designed to serve a specific purpose in the hydraulic fracturing fluid.[1]

Adsorption: Adhesion of molecules of gas, liquid, or dissolved solids to a surface. (U.S. EPA, 2013d)

Advection: A mechanism for moving chemicals in flowing water, where a chemical moves along with the flow of the water itself.

Aeration: A process that promotes biological degradation of organic matter in water. The process may be passive (as when waste is exposed to air) or active (as when a mixing or bubbling device introduces the air). (U.S. EPA, 2013d)

Aerobic mesophiles: Microorganisms that use oxygen for energy production and are tolerant of moderate temperatures.

Analyte: The element, ion, or compound that an analysis seeks to identify; the compound of interest. (U.S. EPA, 2013d)

Annulus: Refers to either the space between the casing of a well and the wellbore or the space between any two strings of tubing or casing. (U.S. EPA, 2013d)

API number: A unique identifying number for all oil and gas wells drilled in the United States. The system was developed by the American Petroleum Institute. (Oil and Gas Mineral Services, 2010)

Aquifer: An underground geological formation, or group of formations, containing water. A source of ground water for wells and springs. (U.S. EPA, 2013d)

Base fluid: The fluid into which additives and proppants are mixed to formulate a hydraulic fracturing fluid.

Basin: A depression in the crust of the earth, caused by plate tectonic activity and subsidence, in which sediments accumulate. Sedimentary basins vary from bowl-shaped to elongated troughs. Basins can be bounded by faults. Rift basins are commonly symmetrical; basins along continental margins tend to be asymmetrical. If rich hydrocarbon source rocks occur in combination with appropriate depth and duration of burial, then a petroleum system can develop within the basin.

[1] Definitions that have no associated citation in this glossary were developed for this assessment.

Most basins contain some amount of shale, thus providing opportunities for shale gas exploration and production. (Schlumberger, 2014)

Biogenic: Methane that is produced in shallower formations by bacterial activity in anaerobic conditions. It is the ultimate dissimilation product of microbially mediated reactions of organic molecules.

Blowout preventer (BOP): Casinghead equipment that prevents the uncontrolled flow of oil, gas, and mud from the well by closing around the drill pipe or sealing the hole. (Oil and Gas Mineral Services, 2010)

Brackish water: Mixed fresh and salt waters. Used here to qualitatively refer to water that contains higher total dissolved solids (TDS) than that typically used for fresh drinking water.

BTEX: An acronym for benzene, toluene, ethylbenzene, and xylenes. These chemicals are a group of single ringed aromatic hydrocarbon based on the benzene structure. These compounds are found in petroleum and are of specific importance because of their health effects.

Caliper log: A log that is used to check for any wellbore irregularities. It is run prior to primary cementing as a means of calculating the amount of cement needed. Also run in conjunction with other open hole logs for log corrections or run on cased holes to evaluate metal loss. (NYSDEC, 2011)

Capillarity: The action by which the surface of a liquid where it is in contact with a solid is elevated or depressed depending on the relative attraction of the molecules of the liquid for each other and for those of the solid. Capillary forces arise from the differential attraction between immiscible fluids and solid surfaces; these are the forces responsible for capillary rise in small-diameter tubes and porous materials. (Adapted from Dake, 1978)

Casing: Steel pipe that is lowered into a wellbore. Casing extends from the bottom of the hole to the surface. (Schlumberger, 2014)

Casing inspection logs: An in situ record of casing thickness and integrity, to determine whether and to what extent the casing has undergone corrosion. The term refers to an individual measurement, or a combination of measurements using acoustic, electrical, and mechanical techniques, to evaluate the casing thickness and other parameters. The log is usually presented with the basic measurements and an estimate of metal loss. It was first introduced in the early 1960s. Today the terms casing-evaluation log and pipe-inspection log are used synonymously. (Schlumberger, 2014)

Cation exchange capacity: The total amount of cations (positively charged ions) that a soil can hold.

Cement: Material used to support and seal the well casing to the rock formations exposed in the borehole. Cement also protects the casing from corrosion and prevents movement of injectate up the borehole. (U.S. EPA, 2013d)

Cement squeeze: A remedial cementing operation designed to force cement into leak paths in wellbore tubulars. The required squeeze pressure is achieved by carefully controlling pump pressure. Squeeze cementing operations may be performed to repair poor primary cement jobs, isolate perforations, or repair damaged casing or liner. (Schlumberger, 2014)

Centralized waste treatment facility (CWT): any facility that treats (for disposal, recycling or recovery of material) any hazardous or non-hazardous industrial wastes, hazardous or non-hazardous industrial wastewater, and/or used material received from off-site. (U.S. EPA, 2012b)

Coalbed methane: Methane contained in coal seams. A coal seam is a layer or stratum of coal parallel to the rock stratification. (U.S. EPA, 2013d)

Collapse pressure: The pressure at which a tube, or vessel, will catastrophically deform as a result of differential pressure acting from outside to inside of the vessel or tube. (Schlumberger, 2014)

Collar: A threaded coupling used to join two lengths of pipe such as production tubing, casing, or liner. The type of thread and style of collar varies with the specifications and manufacturer of the tubing. (Schlumberger, 2014)

Combination truck: A truck tractor or a truck tractor pulling any number of trailers. (U.S. Department of Transportation, 2012)

Community water systems: Public water systems that supply water to the same population year-round. (U.S. EPA, 2013c)

Completion: A term used to describe the assembly of equipment at the bottom of the well that is needed to enable production from an oil or gas well. It can also refer to the activities and methods (including hydraulic fracturing) used to prepare a well for production following drilling.

Complexation: A reaction between two chemicals that form a new complex, either through covalent bonding or ionic forces. This often results in one chemical solubilizing the other.

Compressive strength: Measure of the ability of a substance to withstand compression. (NYSDEC, 2011)

Conductor casing: This large diameter casing is usually the first string of casing in a well. It is set or driven into the unconsolidated material where the well will be drilled to keep the loose material from caving in. (NYSDEC, 2011)

Confidential business information (CBI): Information that contains trade secrets, commercial or financial information, or other information that has been claimed as confidential by the submitter. The EPA has special procedures for handling such information. (U.S. EPA, 2013d)

Contaminant: A substance that is either present in an environment where it does not belong or is present at levels that might cause harmful (adverse) health effects. (U.S. EPA, 2013d)

Conventional reservoir: A reservoir in which buoyant forces keep hydrocarbons in place below a sealing caprock. Reservoir and fluid characteristics of conventional reservoirs typically permit oil or natural gas to flow readily into wellbores. The term is used to make a distinction from shale and other unconventional reservoirs, in which gas might be distributed throughout the reservoir at the basin scale, and in which buoyant forces or the influence of a water column on the location of hydrocarbons within the reservoir are not significant. (Schlumberger, 2014)

Crosslinked gels: linear gels that are linked together by chemicals called crosslinkers, which may link two or more chains together.

Crude oil: A general term for unrefined petroleum or liquid petroleum. (Schlumberger, 2014)

Cumulative effects: Refers to combined changes in the environment that can take place as a result of multiple activities over time and/or space.

Cumulative water use/cumulative water: Refers to the amount of water used or consumed by all hydraulic fracturing wells in a given area per year.

Cyclical stress: Refers to stress caused by frequent or rapid changes in temperature or pressure.

Deviated well: Any non-horizontal well in which the well bottom is intentionally located at a distance (e.g., hundreds of feet) laterally from the wellhead.

Discharge: Any emission (other than natural seepage), intentional or unintentional. Includes, but is not limited to, spilling, leaking, pumping, pouring, emitting, emptying, or dumping. (U.S. EPA, 2013d)

Disinfection byproduct (DBP): A compound formed by the reaction of a disinfectant such as chlorine with organic material in the water supply. (U.S. EPA, 2013d)

Domestic water use: Includes indoor and outdoor water uses at residences, and includes uses such as drinking, food preparation, bathing, washing clothes and dishes, flushing toilets, watering lawns and gardens, and maintaining pools. (USGS, 2015)

Drill bit: The tool used to crush or cut rock. Most bits work by scraping or crushing the rock as part of a rotational motion, while some bits work by pounding the rock vertically. (Schlumberger, 2014)

Drill collar: A component of a drill string that provides weight on the bit for drilling. Drill collars are thick-walled tubular pieces machined from solid bars of steel, usually plain carbon steel but sometimes of nonmagnetic nickel-copper alloy or other nonmagnetic premium alloys. (Schlumberger, 2014)

Drill cuttings: Ground rock produced by the drilling process.

Drill string: The combination of the drillpipe, the bottomhole assembly, and any other tools used to make the drill bit turn at the bottom of the wellbore. (Schlumberger, 2014)

Drilling fluid: Any of a number of liquid and gaseous fluids and mixtures of fluids and solids used when drilling boreholes. (Adapted from Schlumberger, 2014)

Drinking water resource: Any body of ground water or surface water that now serves, or in the future could serve, as a source of drinking water for public or private use (U.S. EPA, 2013d)

Dry gas: Refers to natural gas that occurs in the absence of liquid hydrocarbons. (Adapted from Schlumberger, 2014)

Effluent: Waste material being discharged into the environment, either treated or untreated. (U.S. EPA, 2013d)

Facultative anaerobes: Microorganisms that can use oxygen for energy production if it is present in their environment, but can also use alternatives for energy production if no oxygen is present.

Fault: A fracture or fracture zone along which there has been displacement of the sides relative to each other. (NYSDEC, 2011)

Field: Area of oil and gas production with at least one common reservoir for the entire area. (Oil and Gas Mineral Services, 2010)

Flowback: The term is defined multiple ways in the literature. In general, it is either fluids predominantly containing hydraulic fracturing fluid that return from a well to the surface or a process used to prepare the well for production.

Fluid: A substance that flows when exposed to an external pressure; fluids include both liquids and gases.

Fluid formulation: The entire suite of chemicals, proppant, and base fluid injected into a well during hydraulic fracturing. (U.S. EPA, 2013d)

Formation: A body of earth material with distinctive and characteristic properties and a degree of homogeneity in its physical properties. (U.S. EPA, 2013d)

Formation packer: A specialized casing part that has the same inner diameter as the casing but whose outer diameter expands to make contact with the formation and seal the annulus between the casing and formation, preventing migration of fluids.

Formation fluid: Fluid that occurs naturally within the pores of rock. These fluids consist primarily of water, with varying concentrations of total dissolved solids, but may also contain oil or gas. Sometimes referred to as native fluids, native brines, or reservoir fluids.

FracFocus Registry: A registry for oil and gas well operators to disclose information about hydraulic fracturing well locations, and water and chemical use during hydraulic fracturing

operations developed by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission.

Fracture: A crack or breakage surface within a rock.

Fracture geometry: Refers to characteristics of the fracture such as height and aperture (width).

Fresh water: Qualitatively refers to water with relatively low TDS that is most readily available for drinking water currently.

Gelled fluids: Fracturing fluids that are usually water-based with added gels to increase the fluid viscosity to aid in the transport of proppants. (Spellman, 2012; Gupta and Valkó, 2007)

Ground water: In the broadest sense, all subsurface water; more commonly that part of the subsurface water in the saturated zone. (Solley et al., 1998)

Halite: A soft, soluble evaporate mineral commonly known as salt or rock salt. Can be critical in forming hydrocarbon traps and seals because it tends to flow rather than fracture during deformation, thus preventing hydrocarbons from leaking out of a trap even during and after some types of deformation. (Schlumberger, 2014)

Hazard evaluation: A component of risk assessment that involves gathering and evaluating data on the types of health injuries or diseases (e.g., cancer) that may be produced by a chemical and on the conditions of exposure under which such health effects are produced.

Hazard identification: A process for determining if a chemical or a microbe can cause adverse health effects in humans and what those effects might be. (U.S. EPA, 2013d)

Henry's law constant: Ratio of a chemical's vapor pressure in the atmosphere to its solubility in water. The higher the Henry's law constant, the more volatile the compound will be from water. (NYSDEC, 2011)

Horizontal drilling: Drilling a portion of a well horizontally to expose more of the formation surface area to the wellbore. (Oil and Gas Mineral Services, 2010)

Horizontal well: A well that is drilled vertically up to a point known as the kickoff point, where the well turns toward the horizontal, extending into and parallel with the approximately horizontal targeted producing formation.

Hydraulic fracturing: A stimulation technique used to increase production of oil and gas. Hydraulic fracturing involves the injection of fluids under pressures great enough to fracture the oil- and gas-production formations. (U.S. EPA, 2011a)

Hydraulic fracturing fluids: Engineered fluids, typically consisting of a base fluid, additives, and proppant, that are pumped under high pressure into the well to create and hold open fractures in the formation.

Hydraulic fracturing wastewater: Flowback and produced water that is managed using practices that include but are not limited to reuse in subsequent hydraulic fracturing operations, treatment and discharge, and injection into disposal wells.

Hydraulic fracturing water cycle: The cycle of water in the hydraulic fracturing process, encompassing the acquisition of water, chemical mixing of the fracturing fluid, injection of the fluid into the formation, the production and management of flowback and produced water, and the ultimate treatment and disposal of hydraulic fracturing wastewaters.

Hydraulic gradient: Slope of a water table or potentiometric surface. More specifically, change in the hydraulic head per unit of distance in the direction of the maximum rate of decrease. (U.S. EPA, 2013d)

Hydrocarbon: An organic compound containing only hydrogen and carbon, often occurring in petroleum, natural gas, and coal. (U.S. EPA, 2013d)

Hydrostatic pressure: The pressure exerted by a column of fluid at a given depth.

Imbibition: The displacement of a non-wet fluid (i.e., gas) by a wet fluid (typically water). (Adapted from Dake, 1978)

Immiscible: The chemical property in which two or more liquids or phases are incapable of attaining homogeneity. (U.S. EPA, 2013d)

Impact: Any observed change in the quality or quantity of drinking water resources, regardless of severity, that results from a mechanism.

Impact, potential: Any change in the quality or quantity of drinking water resources that could logically occur, but has not yet been observed, as the result of a mechanism or potential mechanism.

Induced fracture: A fracture created during hydraulic fracturing.

Injection well: A well into which fluids are being injected (40 CFR 144.3).

Integrated risk information system (IRIS): An electronic database that contains the EPA's latest descriptive and quantitative regulatory information about chemical constituents. Files on chemicals maintained in IRIS contain information related to both noncarcinogenic and carcinogenic health effects. (U.S. EPA, 2013d)

Intermediate casing: Casing that seals off intermediate depths and geologic formations that may have considerably different reservoir pressures than deeper zones to be drilled. (Devereux, 1998; Baker, 1979)

Karst: A type of topography that results from dissolution and collapse of carbonate rocks, such as limestone, dolomite, and gypsum, and that is characterized by closed depressions or sinkholes, caves, and underground drainage. (Solley et al., 1998)

Kill fluid: A weighted fluid with a density that is sufficient to overcome the formation pressure and prevent fluids from flowing up the wellbore.

Large truck: A truck with a gross vehicle weight rating greater than 10,000 pounds. (U.S. Department of Transportation, 2012)

Lateral: A horizontal section of a well.

Leakoff: The fraction of the injected fluid that infiltrates into the formation (e.g., through an existing natural fissure) and is not recovered during production.

Linear gel: a series of chemicals linked together so that they form a chain.

Liner: A casing string that does not extend to the top of the wellbore, but instead is anchored or suspended from inside the bottom of the previous casing string. (Schlumberger, 2014)

Lost cement: Refers to a failure of the cement to be circulated back to the surface, indicating that the cement has escaped into the formation.

Lowest-observable-adverse effect level (LOAEL): The lowest exposure level at which there are biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group.

Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are enforceable standards. (U.S. EPA, 2014b)

Mechanical integrity: The absence of significant leakage within the injection tubing, casing, or packer (known as internal mechanical integrity), or outside of the casing (known as external mechanical integrity). (U.S. EPA, 2013d)

Mechanism: A means or series of events by which an activity within the hydraulic fracturing water cycle has been observed to change the quality or quantity of drinking water resources.

Mechanism, potential: A means or series of events by which hydraulic fracturing activities could logically or theoretically (for instance, based on modeling) change the quality or quantity of drinking water resources but one that has not yet been observed.

Mechanism, suspected: A means or series of events by which hydraulic fracturing activities could logically have resulted in an observed change in the quality or quantity of drinking water resources. Available evidence may or may not be sufficient to determine if it is the *only* mechanism that caused the observed change.

Metropolitan combined statistical area: A core urban area of 50,000 or more people. (U.S. Census Bureau, 2013)

Microaerophiles: Microorganisms that require small amounts of oxygen for energy production.

Microannuli: Very small channels that form in the cement and that may serve as pathways for fluid migration to drinking water resources.

Micropolitan combined statistical area: An urban core of at least 10,000, but less than 50,000, people. (U.S. Census Bureau, 2013)

Microseismic monitoring: A technique to track the propagation of a hydraulic fracture as it advances through a formation. (Schlumberger, 2014)

Minimum risk level (MRL): An estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic).

Mobility: The ratio of effective permeability to phase viscosity. The overall mobility is a sum of the individual phase viscosities. Well productivity is directly proportional to the product of the mobility and the layer thickness product. (Schlumberger, 2014)

National Pollution Discharge Elimination System (NPDES): A national program under Section 402 of the Clean Water Act for regulation of discharges of pollutants from point sources to waters of the United States. Discharges are illegal unless authorized by an NPDES permit. (U.S. EPA, 2013d)

National Secondary Drinking Water Regulations (NSDWR): Non-enforceable guidelines regulating contaminants that may cause cosmetic effects (such as skin or tooth discoloration) or aesthetic effects (such as taste, odor, or color) in drinking water (also referred to as secondary standards). (U.S. EPA, 2014b)

Natural gas: A naturally occurring mixture of hydrocarbon and nonhydrocarbon gases in porous formations beneath the earth's surface, often in association with petroleum. The principal constituent of natural gas is methane. (Schlumberger, 2014)

Natural organic matter (NOM): Complex organic compounds that are formed from decomposing plant animal and microbial material in soil and water. (U.S. EPA, 2013d)

Non-community water systems: Water systems that supply water to at least 25 of the same people at least six months per year, but not year-round. (U.S. EPA, 2013c)

Octanol-water partition coefficient (K_{ow}): A coefficient representing the ratio of the solubility of a compound in octanol (a nonpolar solvent) to its solubility in water (a polar solvent). The higher the K_{ow}, the more nonpolar the compound. Log K_{ow} is generally used as a relative indicator of the

tendency of an organic compound to adsorb to soil. Log K_{ow} values are generally inversely related to aqueous solubility and directly proportional to molecular weight. (U.S. EPA, 2013d)

Offset well: An existing wellbore close to a proposed well that provides information for planning the proposed well. (Schlumberger, 2014)

Open hole completion: A well completion that has no casing or liner set across the reservoir formation, allowing the produced fluids to flow directly into the wellbore. (Schlumberger, 2014)

Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

Organic carbon-water partition coefficient (K_{oc}): A coefficient representing the amount of a compound that is adsorbed to soil to the amount of a compound that is dissolved in water, normalized to the total organic carbon content of the soil. The higher the K_{oc}, the more likely a compound is to adsorb to soils and sediments, and the less likely it is to migrate with water. Along with log K_{ow}, log K_{oc} is used as a relative indicator of the tendency of an organic compound to adsorb to soil.

Orphaned well: An inactive oil or gas well with no known (or financially solvent) owner.

Overburden: Material of any nature, consolidated or unconsolidated, that overlies a deposit of useful minerals or ores. (U.S. EPA, 2013d)

Packer: A device that can be run into a wellbore with a smaller initial outside diameter that then expands externally to seal the wellbore. (Schlumberger, 2014)

Pad fluid: a mixture of base fluid, typically water and additives designed to create, elongate, and enlarge fractures along the natural channels of the formation when injected under high pressure.

Partial cementing: Cementing a casing string along only a portion of its length.

Passby flow: A prescribed, low-streamflow threshold below which withdrawals are not allowed. (U.S. EPA, 2015d)

Peer review: A documented critical review of a specific major scientific and/or technical work product. Peer review is intended to uncover any technical problems or unresolved issues in a preliminary or draft work product through the use of independent experts. This information is then used to revise the draft so that the final work product will reflect sound technical information and analyses. The process of peer review enhances the scientific or technical work product so that the decision or position taken by the EPA, based on that product, has a sound and credible basis. (U.S. EPA, 2013d)

Perforation: The communication tunnel created from the casing or liner into the reservoir formation through which injected fluids and oil or gas flows. Also refers to the process of creating communication channels, e.g., via the use of a jet perforating gun.

Permeability: The ability of a material (e.g., rock or soil) to transmit fluid to move through pore spaces.

Persistence: The length of time a compound stays in the environment, once introduced. A compound may persist for less than a second or indefinitely.

Physicochemical properties: The inherent physical and chemical properties of a molecule such as boiling point, density, physical state, molecular weight, vapor pressure, etc. These properties define how a chemical interacts with its environment. (U.S. EPA, 2013d)

Play: A set of oil or gas accumulations sharing similar geologic, geographic properties, such as source rock, hydrocarbon type, and migration pathways. (Oil and Gas Mineral Services, 2010)

Poisson's ratio: A ratio of transverse-to-axial (or latitudinal-to-longitudinal) strain; characterizes how a material is deformed under pressure.

Polar molecule: A molecule with a slightly positive charge at one part of the molecule and a slightly negative charge on another. The water molecule, H2O, is an example of a polar molecule, where the molecule is slightly positive around the hydrogen atoms and negative around the oxygen atom.

Porosity: A measure of pore space, or the percentage of the material (e.g., rock or soil) volume that can be occupied by oil, gas, or water.

Produced water: Water that flows from oil and gas wells.

Production casing: The deepest casing set and serves primarily as the conduit for producing fluids, although when cemented to the wellbore, this casing can also serve to seal off other subsurface zones including ground water resources. (Devereux, 1998; Baker, 1979)

Production well: A well that is used to bring fluids (such as oil or gas) to the surface.

Production zone: Refers to the portion of a subsurface rock zone that contains oil or gas to be extracted (sometimes using hydraulic fracturing). The production zone is sometimes referred to as the target zone.

Proppant/propping agent: A granular substance (sand grains, aluminum pellets, or other material) that is carried in suspension by the fracturing fluid and that serves to keep the cracks open when fracturing fluid is withdrawn after a fracture treatment. (U.S. EPA, 2013d)

Protected ground water resource: The deepest aquifer that the state or other regulatory agency requires to be protected from fluid migration through or along wellbores.

Public water system source: The source of the surface or ground water used by a public water system, including source wells, intakes, reservoirs, infiltration galleries, and springs.

Public water systems: Water systems that provide water for human consumption from surface or ground water through pipes or other infrastructure to at least 15 service connections or serve an average of at least 25 people for at least 60 days a year. (Safe Drinking Water Act, 2002)

Publicly owned treatment works (POTW): Any device or system used in the treatment (including recycling and reclamation) of municipal sewage or industrial wastes of a liquid nature that is owned by a state or municipality. This definition includes sewers, pipes, or other conveyances only if they convey wastewater to a POTW providing treatment. (U.S. EPA, 2013d)

Quality assurance (QA): An integrated system of management activities involving planning, implementation, documentation, assessment, reporting, and quality improvement to ensure that a process, item, or service is of the type and quality needed and expected by the customer. (U.S. EPA, 2013d)

Quality assurance project plan (QAPP): A formal document describing in comprehensive detail the necessary quality assurance procedures, quality control activities, and other technical activities that need to be implemented to ensure that the results of the work performed will satisfy the stated performance or acceptance criteria. (U.S. EPA, 2013d)

Quality management plan: A document that describes a quality system in terms of the organizational structure, policy and procedures, functional responsibilities of management and staff, lines of authority, and required interfaces for those planning, implementing, documenting, and assessing all activities conducted. (U.S. EPA, 2013d)

Radioactive tracer log: A record of the presence of tracer material placed in or around the borehole to measure fluid movement in injection wells. (Schlumberger, 2014)

Radionuclide: Radioactive particle, man-made or natural, with a distinct atomic weight number. Emits radiation in the form of alpha or beta particles, or as gamma rays. Can have a long life as soil or water pollutant. Prolonged exposure to radionuclides increases the risk of cancer. (U.S. EPA, 2013d)

Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime.

Reference value (RfV): An estimate of an exposure for a given duration to the human population (including susceptible subgroups) that is likely to be without an appreciable risk of adverse health effects over a lifetime. Reference value is a generic term not specific to a given route of exposure.

Relative permeability: A dimensionless property allowing for comparison of the different abilities of fluids to flow in multiphase settings. If a single fluid is present, its relative permeability is equal

to 1, but the presence of multiple fluids generally inhibits flow and decreases the relative permeability.

Reservoir: A porous and permeable geologic formation where hydrocarbons collect under pressure over geological time.

Residuals: The solids generated or retained during the treatment of wastewater. (U.S. EPA, 2013d)

Safe Drinking Water Act (SDWA): The act designed to protect the nation's drinking water supply by establishing national drinking water standards (maximum contaminant levels or specific treatment techniques) and by regulating underground injection control wells. (U.S. EPA, 2013d)

Sandstone: A clastic sedimentary rock whose grains are predominantly sand sized. The term is commonly used to imply consolidated sand or a rock made of predominantly quartz sand, although sandstones often contain feldspar, rock fragments, mica, and numerous additional mineral grains held together with silica or another type of cement. The relatively high porosity and permeability of sandstones make them good reservoir rocks. (Schlumberger, 2014)

Science Advisory Board (SAB): A federal advisory committee that provides a balanced, expert assessment of scientific matters relevant to the EPA. An important function of the Science Advisory Board is to review EPA's technical programs and research plans. (U.S. EPA, 2013d)

Service company: A company that assists well operators by providing specialty services, including hydraulic fracturing. (U.S. EPA, 2013d)

Shale: A fine-grained, fissile, detrital sedimentary rock formed by consolidation of clay- and silt-sized particles into thin, relatively impermeable layers. (Schlumberger, 2014)

Shale gas: Natural gas generated and stored in shale.

Shale oil: Oil present in unconventional oil reservoirs that are made up of shale.

Shut-in: The process of sealing off a well by either closing the valves at the wellhead, a downhole safety valve, or a blowout preventer.

Slickwater: A type of fracturing fluid that consists mainly of water with a very low portion of additives like polymers that serve as friction reducers to reduce friction loss when pumping the fracturing fluid downhole. (Barati and Liang, 2014)

Solubility: The amount of mass of a compound that will dissolve in a unit volume of solution. (U.S. EPA, 2013d)

Sorption: The general term used to describe the partitioning of a chemical between soil and water and depends on the nature of the solids and the properties of the chemical.

Source water: Surface or ground water, or reused wastewater, acquired for use in hydraulic fracturing. (U.S. EPA, 2013d)

Spacer fluid: A fluid pumped before the cement to clean drilling mud out of the wellbore.

Spud (spud a well): To start the well drilling process by removing rock, dirt, and other sedimentary material with the drill bit. (U.S. EPA, 2013d)

Stages (frac stages): A single reservoir interval that is hydraulically stimulated in succession with other intervals.

Stimulation: Refers to (1) injecting fluids to clear the well or pore spaces near the well of drilling mud or other materials that create blockage and inhibit optimal production (i.e., matrix treatment) and (2) injecting fluid to fracture the rock to optimize the production of oil or gas.

Stray gas: Refers to the phenomenon of natural gas (primarily methane) migrating into shallow drinking water resources or to the surface.

Strings: An assembled length of steel pipe configured to suit a specific wellbore.

Subsurface formation: A mappable body of rock of distinctive rock type(s), including the rock's pore volume (i.e., the void space within a formation that fluid flow can occur, as opposed to the bulk volume which includes both pore and solid phase volume), with a unique stratigraphic position.

Surface casing: The shallowest cemented casing, with the widest diameter. Cemented surface casing generally serves as an anchor for blowout protection equipment and to seal off drinking water resources. (Baker, 1979)

Surface water: All water naturally open to the atmosphere (rivers, lakes, reservoirs, ponds, streams, impoundments, seas, estuaries, etc.). (U.S. EPA, 2013d)

Surfactant: Used during the hydraulic fracturing process to decrease liquid surface tension and improve fluid passage through the pipes. (U.S. EPA, 2013d)

Sustained casing pressure: Refers to cases when the pressure in any well annulus that is measurable at the wellhead rebuilds after it is bled down, not caused solely by temperature fluctuations or imposed by the operator. If the pressure is relieved by venting natural gas from the annulus to the atmosphere, it will build up again once the annulus is closed (i.e., the pressure is sustained). (Skjerven et al., 2011)

Technically recoverable resources: The volumes of oil and natural gas that could be produced with current technology, regardless of oil and natural gas prices and production costs. (EIA, 2013)

Temperature log: A log of the temperature of the fluids in the borehole; a differential temperature log records the rate of change in temperature with depth and is sensitive to very small changes. (U.S. EPA, 2013d)

Tensile strength: The force per unit cross-sectional area required to pull a substance apart. (Schlumberger, 2014)

Thermogenic: Methane that is produced by high temperatures and pressures in deep formations over geologic timescales. Thermogenic methane is formed by the thermal breakdown, or cracking, of organic material that occurs during deep burial of sediment.

Tight oil: Oil found in relatively impermeable reservoir rock. (Schlumberger, 2014)

Total dissolved solids (TDS): The quantity of dissolved material in a given volume of water. Total dissolved solids can include salts (e.g., sodium chloride), dissolved metals, radionuclides, and dissolved organics. (U.S. EPA, 2013d)

Toxicity: The degree to which a substance or mixture of substances can harm humans or animals. Acute toxicity involves harmful effects in an organism through a single or short-term exposure. Chronic toxicity is the ability of a substance or mixture of substances to cause harmful effects over an extended period, usually upon repeated or continuous exposure, sometimes lasting for the entire life of the exposed organism. Subchronic toxicity is the ability of the substance to cause effects for more than 1 year but less than the lifetime of the exposed organism. (U.S. EPA, 2013d)

Tubing: The narrowest casing set within a completed well, either hung directly from the wellhead or secured at its bottom using a packer. Tubing is not typically cemented in the well.

Unconventional reservoir: A reservoir characterized by lower permeability than conventional reservoirs. It can be the same formation where hydrocarbons are formed and also serve as the source for hydrocarbons that migrate and accumulate in conventional reservoirs. Unconventional reservoirs can include methane-rich coalbeds and oil- and/or gas-bearing shales and tight sands.

Unconventional resource: An umbrella term for oil and natural gas that is produced by means that do not meet the criteria for conventional production. What has qualified as unconventional at any particular time is a complex function of resource characteristics, the available exploration and production technologies, the economic environment, and the scale, frequency, and duration of production from the resource. Perceptions of these factors inevitably change over time and often differ among users of the term. At present, the term is used in reference to oil and gas resources whose porosity, permeability, fluid trapping mechanism, or other characteristics differ from conventional sandstone and carbonate reservoirs. Coalbed methane, gas hydrates, shale gas, fractured reservoirs, and tight gas sands are considered unconventional resources. (Schlumberger, 2014)

Underground Injection Control (UIC): The program under the Safe Drinking Water Act that regulates the use of wells to pump fluids into the ground. (U.S. EPA, 2013d)

Unsaturated zone: The soil zone above the water table that is only partially filled by water; also referred to as the "vadose zone."

Vapor pressure: The force per unit area exerted by a vapor in an equilibrium state with its pure solid, liquid, or solution at a given temperature. Vapor pressure is a measure of a substance's

propensity to evaporate. Vapor pressure increases exponentially with an increase in temperature. (U.S. EPA, 2013d)

Vertical well: A well in which the wellbore is vertical throughout its entire length, from the wellhead at the surface to the production zone.

Viscosity: A measure of the internal friction of a fluid that provides resistance to shear within the fluid, informally referred to as how "thick" a fluid is.

Volatile: Readily vaporizable at a relatively low temperature. (U.S. EPA, 2013d)

Volatilization: The process in which a chemical leaves the liquid phase and enters the gas phase.

Wastewater treatment: Chemical, biological, and mechanical procedures applied to an industrial or municipal discharge or to any other sources of contaminated water in order to remove, reduce, or neutralize contaminants. (U.S. EPA, 2013d)

Water availability: There is no standard definition for water availability, and it has not been assessed recently at the national scale (U.S. GAO, 2014). Instead, a number of water availability indicators have been suggested (e.g., Roy et al., 2005). Here, availability is most often used to qualitatively refer to the amount of a location's water that could, currently or in the future, serve as a source of drinking water (U.S. GAO, 2014), which is a function of water inputs to a hydrologic system (e.g., rain, snowmelt, groundwater recharge) and water outputs from that system occurring either naturally or through competing demands of users.

Water consumption: Water that is removed from the local hydrologic cycle following its use (e.g., via evaporation, transpiration, incorporation into products or crops, consumption by humans or livestock), and is therefore unavailable to other water users (Maupin et al., 2014).

Water intensity: The amount of water used per unit of energy obtained. (Nicot et al., 2014; Laurenzi and Jersey, 2013)

Water reuse: Any hydraulic fracturing wastewater that is used to offset total fresh water withdrawals for hydraulic fracturing, regardless of the level of treatment required.

Water use: Water withdrawn for a specific purpose, part or all of which may be returned to the local hydrologic cycle.

Water withdrawal: Water removed from the ground or diverted from a surface-water source for use. (Nicot et al., 2014; Laurenzi and Jersey, 2013)

Well blowout: The uncontrolled flow of fluids out of a well.

Well communication: Refers to fractures intersecting abandoned or active (producing) offset wells near the well that is being stimulated.

Well logging: A continuous measurement of physical properties in or around the well with electrically powered instruments to infer formation properties. Measurements may include electrical properties (resistivity and conductivity), sonic properties, active and passive nuclear measurements, measurements of the wellbore, pressure measurement, formation fluid sampling, sidewall coring tools, and others. Measurements may be taken via a wireline, which is a wire or cable that is used to deploy tools and instruments downhole and that transmits data to the surface. (Adapted from Schlumberger, 2014)

Well operator: A company that controls and operates oil and gas wells. (U.S. EPA, 2013d)

Well pad: A temporary drilling site, usually constructed of local materials such as sand and gravel. After the drilling operation is over, most of the pad is usually removed or plowed back into the ground. (NYSDEC, 2011)

Wellbore: The drilled hole or borehole, including the open hole or uncased portion of the well.

Wet gas: Refers to natural gas that typically contains less than 85% methane along with ethane and more complex hydrocarbons.

Wetting/nonwetting: The preferential attraction of a fluid to the surface. In typical reservoirs, water preferentially wets the surface, and gas is nonwetting. (Adapted from Dake, 1978)

Workover: Refers to any maintenance activity performed on a well that involves ceasing operations and removing the wellhead.

Young's modulus: A ratio of stress to strain that is a measure of the rigidity of a material.

J.2. References for Appendix J

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