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**HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

**REPORT FOR THE  
DIETHYLBENZENE-RICH STREAMS CATEGORY**

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**American Chemistry Council  
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**April 26, 2004**

## Report for The Diethylbenzene-Rich Streams HPV Category

### EXECUTIVE SUMMARY

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies of the Diethylbenzene-Rich Streams HPV Task Group (Task Group) developed screening level human health, environmental effects and fate, and physicochemical data for the Diethylbenzene-Rich Streams category under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program).

The category is defined as Diethylbenzene-Rich Streams. This category consists of streams that contain a predominance of diethylbenzene isomers and are produced during ethylbenzene manufacture.

Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene, and, to a much lesser extent, further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying limited amounts. After the ethylbenzene is removed, the remaining stream is separated into a diethylbenzene-rich stream and a bottoms stream. Some manufacturers may further process the diethylbenzene-rich streams to increase the diethylbenzene content.

This report for the Diethylbenzene-Rich Streams category addresses two streams that contain a predominance of diethylbenzene isomers (87.6 – 98.8 wt%) and are produced during ethylbenzene manufacture. The range of composition for both Diethylbenzene-Rich Streams (CAS No. 25340-17-4 and CAS No. 68608-82-2) is very similar. For purposes of the testing conducted under this HPV program, equal quantities of the streams from each of the currently producing companies were combined to form a representative test sample of Diethylbenzene-Rich Streams (Diethylbenzene Blend).

#### Physical/Chemical Properties

The boiling point of Diethylbenzene Blend was determined to be  $180.8 \pm 1.7$  °C (Huntley, 2003a). The freezing point of the blend was determined to be  $< -75$  °C (Huntley, 2003b). The tested blend had vapor pressures of 210, 310 and 530 Pa at 10.0, 20.0 and 30.0 °C respectively (Huntley, 2003c). The water solubility of the blend was  $15.7 \pm 1.4$  µg/L in reagent water at 20 °C (Hahn, 2003). The alkylaromatic compounds that constitute the Diethylbenzene-Rich Streams do not undergo direct photolysis or hydrolysis in the environment. Photochemical oxidation via reaction with hydroxyl radicals (indirect photolysis) is relatively rapid. Under average conditions the half-lives of the components of the Diethylbenzene-Rich Streams category range from 0.75-1.5 days.

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### **Environmental Fate/Pathways**

Substances in the Diethylbenzene-Rich Streams category are calculated to partition at equilibrium primarily into air with negligible percentages partitioning in water, soil and sediment. The volatility and low water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. However under steady-state conditions, including transport and degradation, the substances are present predominantly in the compartments into which they are released. Since this material is susceptible to destructive reactions such as indirect photolysis and biodegradation, this material is expected to be short-lived in the environment (5-10 day residence times).

### **Ecotoxicity**

Aquatic toxicity endpoints for the OECD SIDS/HPV Chemical program include acute toxicity to freshwater fish, invertebrate, and alga. These endpoints have been determined (Hicks, 2003a, b, c) for the Diethylbenzene Blend, using static-renewal dosing solutions to maximize solution concentrations for this volatile substance. In such worst-case exposures, the data indicate that diethylbenzene may be categorized using EPA criteria (Zucker, 1985) as “highly toxic” to rainbow trout (*Oncorhynchus mykiss*), based on a 96-hr LC50 value of 0.673 mg a.i./L (Hicks, 2002a). In another static-renewal exposure system, the chemical was found to be “moderately toxic” to the water flea, *Daphnia magna*, with a 48-hr EC50 value of 2.0 mg a.i./L (Hicks, 2002b). Similarly, the 72-hr EC50 values (biomass, growth) for diethylbenzene with the freshwater green algae, *Selenastrum capricornutum*, ranged from 1.0 to 1.2 mg a.i./L ((Hicks, 2002c).

### **Human Health Effects**

Diethylbenzene-rich streams are categorized by low acute oral and dermal toxicity. Oral LD<sub>50</sub> in rats ranging from 2050 to 6900 mg/kg have been reported for Mixed Diethylbenzenes. The acute dermal LD<sub>50</sub> in rats was reported to be greater than 2000 mg/kg in rats and greater than 5000 mg/kg in rabbits.

There are a number of repeated dose, subchronic toxicity studies with Mixed Diethylbenzene and diethylbenzene isomers; some of these studies have focused on neurotoxicity. Rats exposed via inhalation to Mixed Diethylbenzenes at 0, 190, 610 and 1400 mg/m<sup>3</sup> for 10 weeks, six hr/day, five days per week (Kaempfe and Thake, 1993) showed no treatment-related abnormal clinical observations. There were treatment-related changes in some hematologic parameters and in serum chemistry parameters in mid to high exposure groups. Abnormal coloration of brains and urinary bladders of some animals was attributed possibly to the presence of the parent chemical or a metabolite in those tissues. There were no other gross or macroscopic changes attributed to the test

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material, including no effects on reproductive organs of either sex. The NOAEL was 190 mg/m<sup>3</sup>.

Mixed Diethylbenzenes tested negative in a number of *in vitro* genetic toxicity studies (e.g. bacterial mutations, chromosomal aberration in Chinese hamster ovary cells) and *in vivo* assays (e.g. micronuclei in bone marrow erythrocytes).

Mixed Diethylbenzenes does not appear to be a reproductive or developmental toxicant. Mixed Diethylbenzenes administered orally to pregnant rats on gestation days 6-16 at 20, 100 and 200 mg/kg did not cause birth defects or developmental variations (Mercieca, 1992). The NOEL for maternal toxicity (reduced body weights and food consumption) was 20 mg/kg, whereas the NOEL for fetal body weight effects was 100 mg/kg.

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**LIST OF MEMBER COMPANIES**  
**ETHYLBENZENE PANEL**  
**DIETHYLBENZENE HPV TASK GROUP**

BP Amoco Chemical Company

Chevron Phillips Chemical Company LP

The Dow Chemical Company

Koch Specialty Chemical Company; a Division of Koch Petroleum Company

Sterling Chemicals Inc.

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## **Report for The Diethylbenzene -Rich Streams HPV Category**

### **REPORT FOR THE DIETHYLBENZENE-RICH STREAMS CATEGORY**

#### **I. INTRODUCTION**

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies of the Diethylbenzene-Rich Streams HPV Task Group (Task Group) developed screening level human health, environmental effects and fate, and physicochemical data for the Diethylbenzene-Rich Streams category under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program).

For the Diethylbenzene-Rich Streams HPV, the Task Group has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, the Task Group has conducted a thoughtful, qualitative analysis of the adequacy of existing data. The Task Group has taken the same thoughtful approach when developing and implementing its test plan (Ethylbenzene Panel, 2003).

#### **II. DESCRIPTION OF THE DIETHYLBENZENE-RICH STREAMS CATEGORY**

The category was defined as Diethylbenzene-Rich Streams. This category consists of streams that contain a predominance of diethylbenzene isomers and are produced during ethylbenzene manufacture.

Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene, and, to a much lesser extent, further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying limited amounts. After the ethylbenzene is removed, the remaining stream is separated into a diethylbenzene-rich stream and a bottoms stream. Some manufacturers may further process the diethylbenzene-rich streams to increase the diethylbenzene content. The diethylbenzene-rich streams are identified by two CAS Registry Numbers:

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Chemical Name	Other Name	CAS No.
Diethylbenzene	Mixed Diethylbenzenes	25340-17-4
Benzene, ethylenated, by-products from	Polyethylbenzenes	68608-82-2

The composition of both diethylbenzene-rich streams is listed below based on capillary GC analysis of samples submitted by the four participating companies to BP Amoco Analytical Technology (BP Amoco, 2000).

Component	CAS #68608-82-2	CAS # 25340-17-4
	Wt %	Wt%
Diethylbenzenes <sup>1</sup>	87.6 – 89.9	94.3 – 98.8
Triethylbenzenes	4.9 -5.1	<0.1
Polyethylbenzenes	<0.1	<0.1
Iso-/sec-butylbenzenes	1.1	0.6 – 0.8
Other alkylbenzenes	0.7 – 1.8	0.3 – 4.5
Ethylbenzene	1.7 – 1.9	<0.1
Benzene	<0.1	<0.1
Diphenylalkanes	<0.1	<0.1
Ethyl diphenylethanes and Diethyl biphenyls	<0.1	<0.1
PNAs (3-rings)	<0.1	<0.1
Paraffins/Naphthenes	0.5 – 1.6	<0.1
Total of unidentified components, each present at <0.1%	0.2 – 0.6	0.8 – 1.4

<sup>1</sup>n-butylbenzene coeluted with 1,4-diethylbenzene

As shown in the table above, the range of composition for both Diethylbenzene-Rich Streams (CAS No. 25340-17-4 and CAS No. 68608-82-2) are very similar. For purposes of the HPV testing program, equal quantities of the streams from each of current producers were combined to form a representative test sample of Diethylbenzene-Rich Streams (Diethylbenzene Blend).

Please note that the Polyethylbenzene Bottoms (CAS Registry #68987-42-8: benzene, ethylated, residues) is being tested separately under the HPV Chemical Program. For comparison, the composition of the Polyethylbenzene Bottoms is attached as Appendix 2.

### III. SUMMARY OF NEW AND EXISTING INFORMATION

New data (from the HPV testing program conducted) as well as existing information on Diethylbenzene-Rich Streams and diethylbenzene isomers is summarized below. The endpoints with sufficient data for the HPV program are summarized in Appendix 1.

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### A. Physical/Chemical Properties

The HPV Program physicochemical endpoints include: melting point, boiling point, vapor pressure, water solubility, and octanol/water coefficient ( $K_{ow}$ ). Until these tests were conducted, there were only reported data for these endpoints for diethylbenzene isomers but not for Diethylbenzene-Rich Streams (HSDB, 2001).

**Table 1. Summary of available physicochemical data for diethylbenzene isomers (HSDB, 2001)**

	1,2-Diethylbenzene	1,3-Diethylbenzene	1,3-Diethylbenzene
Boiling Point (°C)	184	181.1	183.7
Melting Point (°C)	-31.2	-83.9	-42.83
Vapor Pressure (mm Hg at 25 °C)	1.05 (140 Pa)	1.20 160 Pa	1.03 137 Pa
Water Solubility (mg/l at 25 °C)	71.1	24.0	24.8
Octanol/Water Partition Coeff. (log $K_{ow}$ )	3.72	4.44	4.45

Under the Diethylbenzene-Rich Streams HPV program, the boiling point, freezing point, vapor pressure, and water solubility for a diethylbenzene blend were measured. The tested Diethylbenzene Blend was comprised of equal volumes from three diethylbenzene samples obtained from BP Amoco Chemical Company, The Dow Chemical Company and Sterling Chemicals, Inc.

The boiling point of the tested Diethylbenzene Blend was determined to be  $180.8 \pm 1.7$  °C (Huntley, 2003a). The freezing point of the blend determined was  $< -75$  °C (Huntley, 2003b). The tested blend had vapor pressures of 210, 310 and 530 Pa at 10.0, 20.0 and 30.0 °C respectively (Huntley, 2003c). The water solubility of the blend was  $15.7 \pm 1.4$  mg/L in reagent water at 20 °C (Hahn, 2003).

The table below is a summary of measured physicochemical properties for Diethylbenzene Blend.

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**Table 2. Summary of measured physicochemical properties for tested Diethylbenzene Blend**

Properties	Results for Diethylbenzene Blend
Boiling point	180.8 ± 1.7 °C
Freezing point	< -75 °C
Vapor pressure	?? 210 ± 44Pa at 10 °C ?? 310 ± 35 Pa at 20 °C ?? 530 ±15 Pa at 30 °C
Water Solubility	15.7 ± 1.4 mg/L at 20 °C

The octanol/water partition coefficient was not evaluated due to the technical infeasibility of determination for a stream. Partition coefficients for the constituent isomers (Table 1) were used as surrogates for modeling and other calculations.

### **B. Environmental Fate/Pathways**

Environmental fate endpoints for the HPV Program include: biodegradation, photodegradation, hydrolysis, and fugacity.

#### **1. Biodegradation**

In a CO<sub>2</sub> evolution test using unacclimated microbial cultures, Mixed Diethylbenzenes degraded 4.7% after 28 days and 5.5% after 35 days, indicating that it is not readily biodegradable (Marks et al., 1995). Similar results were obtained for 1,4-diethylbenzene (MITI, 1993; SIDS Dossier, 1994; SIDS SIAR, 1994). However, acclimated microorganisms completely degraded all three isomers of diethylbenzene at low concentrations (< 0.5 mg/l in about 5 days (MHW, 1993c; HSDB, 2001) However the diethylbenzenes in percolation (Kappeler, Th., and Wuhrmann, K., 1978) or sealed flask tests (Kappeler, Th., and Wuhrmann, K., 1978a) at 10 °C with mixed autochthonous flora in clean ground water samples from Tuffenwies and Zurich, Switzerland or in flasks at 20 °C with North Sea coast water (Van der Linden, A. C.,1978) were only a small fraction of the hydrocarbons extracted from gas oil into water. The conclusion is valid only for cooxidation of diethylbenzenes with other hydrocarbons. 1,2-Diethylbenzene was relatively unreactive, requiring 12 days at 10°C (Kappeler, Th., and Wuhrmann, K., 1978a) to vanish. The best estimate of biodegradation is probably the QSAR in BIOWIN version 4.01, (Meylan. and Howard, 2000) a subroutine of EPIWIN version 3.04. Primary biodegradation is defined by disappearance of the compound. Ultimate biodegradation is mineralization (oxidation of intermediates to CO<sub>2</sub>). The prediction for

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all isomers on the rating scale of 4.0 = days; 3.5 = days to weeks, 3.0 = weeks and 2.5 = weeks to months is 3.52 (days-weeks) primary biodegradation and 2.75 (weeks-months) for ultimate biodegradation. Based on the BIOWIN ultimate degradation, adjusted for each compartment and rounded off, a half-life in water of 360 hours; a half-life in soil of 360 hours; and a half-life in sediment of 1440 hours EPIWIN were inputs to the EQC Level III model of environmental fate (Trent University, 2002) run within EPIWIN.

### 2. Photodegradation

**Direct photodegradation:** The absorption of light in the ultraviolet (UV) visible range can induce electronic excitation of an organic molecule. The stratospheric ozone layer allows only light in wavelengths in the 290-750nm range to reach earth's surface with the potential to result in photochemical transformation in the environment. To estimate photochemical degradation, it is assumed that degradation will occur in proportion to the amount of light wavelengths greater than 290 nm absorbed by the molecule. Saturated hydrocarbons (paraffins and naphthenics), olefins with one double bond or two conjugated double bonds, and single ring aromatics do not absorb appreciable light energy above 290nm.

Therefore products in the Diethylbenzene-Rich Streams Category do not contain component molecules that will undergo direct photolysis. This process will not contribute a measurable degradative removal of chemical components in this category from the environment.

**Atmospheric Oxidation (Indirect photodegradation):** Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation but an indirect degradation process. Hydrocarbons such as those in the Diethylbenzene-Rich Streams Category have the potential to volatilize to air where they can react with hydroxyl radicals (OH<sup>-</sup>). The rate at which an organic compound reacts with OH<sup>-</sup> radicals is a direct measure of its atmospheric persistence. The AopWin version 1.91 subroutine of EPIWIN 3.04 (US EPA, 2000) was used to estimate the rate constants for OH<sup>-</sup> radical reactions of representative organic constituents of the products in the Diethylbenzene-Rich Streams category, which are then used to calculate atmospheric half-lives (12-hr days) with  $1.5 \times 10^6$  molecules/cm<sup>3</sup> of HO<sup>•</sup> (global tropospheric daytime average) for these constituents as shown below:

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**Table 3. Indirect photolysis of components of the Diethylbenzene -Rich Streams category**

Chemical	Calculated half-life (hrs)	Estimated OH- Rate Constant (cm <sup>3</sup> /molecule-sec)	OH- Rate Constant (cm <sup>3</sup> /molecule-sec) (Atkinson, R., 1989)
1,2-diethylbenzene	15.8	8.1 x 10 <sup>-12</sup>	
1,3-diethylbenzene	9.0	14.2 x 10 <sup>-12</sup>	
1,4-diethylbenzene	15.8	8.1 x 10 <sup>-12</sup>	
ethylbenzene	18.0		7.1 x 10 <sup>-12</sup>

Based on these calculated values, products in the Diethylbenzene-Rich Streams Category can have an atmospheric half-life range of 0.75-1.5 days (based on a 12-hr day), indicating that atmospheric oxidation can be a significant route of degradation for products in this category.

### 3. Hydrolysis

Hydrolysis is unlikely for product streams in the Diethylbenzene-Rich Streams Category. Hydrolysis is a nucleophilic substitution reaction in which a water molecule or hydroxide ion reacts with an organic molecule to form a new carbon-oxygen bond. Carbon to carbon double bonds are too stable to be cleaved by nucleophilic substitution and the carbon atom lacks sufficient electronegativity to be a good “leaving group”. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters and sulfonic acid esters. The chemical components of the Diethylbenzene-Rich Streams are hydrocarbons that are not included in these groups and have very low potential to hydrolyze. 1,4-Diethylbenzene did not hydrolyze at pH 4, 7 or 9 in 5 days at 50°C (MITI, 1993). This degradative process will not contribute to removal of these hydrocarbons in the environment.

### 4. Chemical Transport and Distribution in the Environment (Fugacity Modeling)

Chemical transport has been assessed using Level I, II and III fugacity models to determine the relative distribution of chemicals between selected environmental compartments (e.g. air, soil, sediment and water). The results from the fugacity modeling for the three major constituents of products in this category (1,2 diethylbenzene, 1,3 diethylbenzene and 1,4 diethylbenzene) indicate that these compounds will partition primarily to air under the equilibrium conditions of Level I and II models (Table 4.)

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**Table 4. Summary of the EQC Level I fugacity model (Mackay et al., 1996) results for 1,2 diethylbenzene, 1,3 diethylbenzene and 1,4 diethylbenzene**

CHEMICAL	Percent Distribution:			
	Air	Water	Soil	Sediment
1,2-Diethylbenzene	99.0	0.18	0.85	0.02
1,3-Diethylbenzene	95.4	0.18	4.3	0.10
1,4-Diethylbenzene	95.3	0.18	4.4	0.10

Volatility and low water solubility largely control the partitioning behavior of constituent chemicals in substances from this category.

However under steady-state conditions, including transport and degradation, the substances are present predominantly in the compartments into which they are released. The EQC Level III Fugacity Model (Trent University, 2002) was used to determine the steady-state fluxes and concentrations of diethylbenzenes with various emission scenarios.

**Table 5. Environmental fate of 1,3-diethylbenzene from an EQC Level III model**

	Air	Water	Soil	Sediment
<b>Emission to Air</b>				
Reaction	7.2.0%	0.0%	0.0%	0.0%
Advection	92.8%	0.0%		0.0%
Relative Concentration	99.6%	0.0%	0.4%	0.0%
<b>Emission to Water</b>				
Reaction	3.2%	18.5%	0.0%	1.9%
Advection	41.4%	34.9%		0.1%
Relative Concentration	0.3%	82.3%	0.0%	17.4%
<b>Emission to Soil</b>				
Reaction	2.1%	0.0%	70.6%	0.0%
Advection	27.2%	0.0%		0.0%
Relative Concentration	0.15%	0.04%	99.8%	0.0%

1,4-Diethylbenzene partitions essentially the same as 1,3-diethylbenzene, but the ortho-substituted compound, 1,2-diethylbenzene, has higher volatility and partitions more into air.

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**Table 6. Environmental fate of 1,2-diethylbenzene from an EQC Level III model**

	Air	Water	Soil	Sediment
<b>Emission to Air</b>				
Reaction	4.2.0%	0.0%	0.0%	0.0%
Advection	95.8%	0.0%		0.0%
Relative Concentration	99.8%	0.0%	0.16%	0.0%
<b>Emission to Water</b>				
Reaction	1.9%	18.5%	0.0%	0.3%
Advection	43.7%	35.5%		0.0%
Relative Concentration	0.5%	96.0%	0.0%	3.5%
<b>Emission to Soil</b>				
Reaction	2.9%	0.1%	31.6%	0.0%
Advection	65.4%	0.0%		0.0%
Relative Concentration	0.8%	0.2%	99.0%	0.0%

Using the default assumption of equal emissions to air, water and soil and the default landscape, the steady-state distributions were estimated to be:

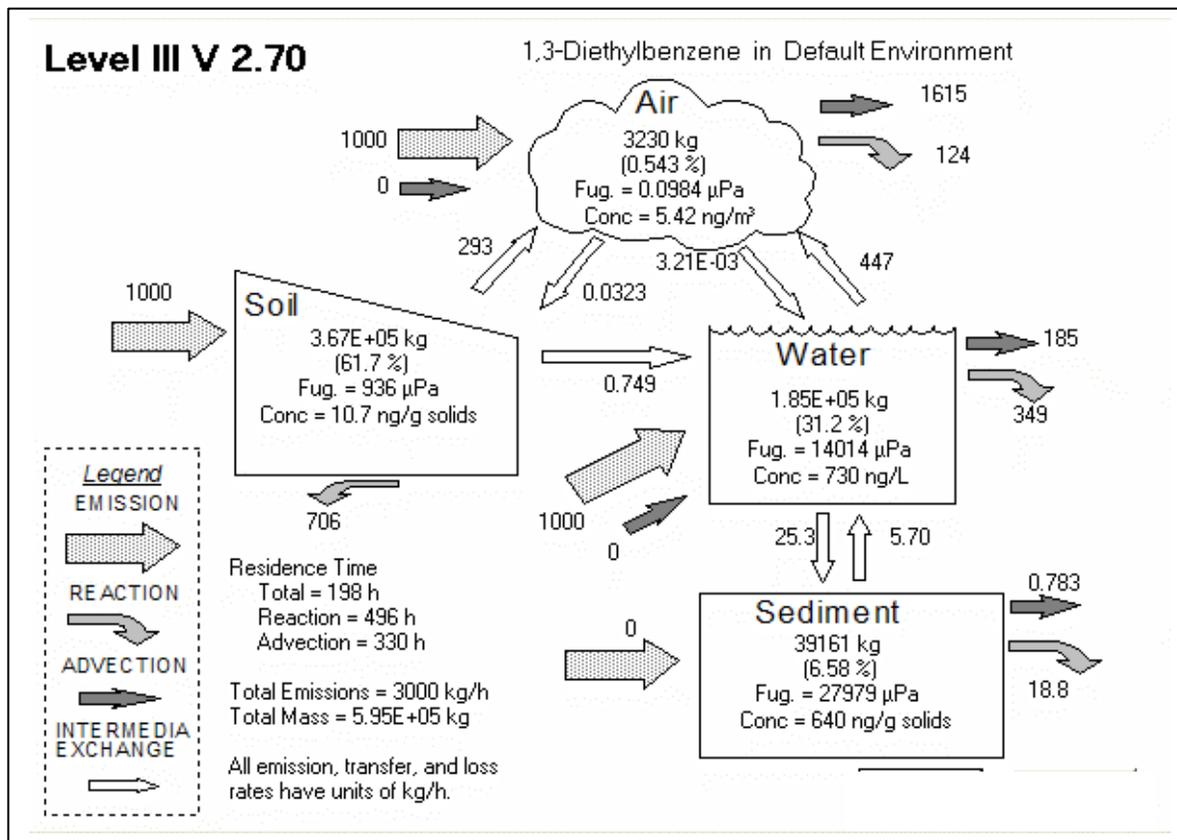
**Table 7. Distribution of diethylbenzenes with equal loading of air, water and soil under default EQC Level III conditions**

CHEMICAL	Percent Distribution:			
	Air	Water	Soil	Sediment
1,2-Diethylbenzene	1.14	51.4	45.5	1.9
1,3-Diethylbenzene	0.54	31.2	61.7	6.6
1,4-Diethylbenzene	0.56	31.0	61.8	6.7

These results reflect the Level III model's loading pattern plus the assumed moderately long half-life in water and soil and short half-life in air. While the hydrocarbons tend to partition into air, the relatively fast rates of advection and reaction in air leave little of the mass there. The processes for 1,3-diethylbenzene are shown diagrammatically below in Figure 1.

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Figure 1. Process description for 1,3-diethylbenzene under EQC Level III fugacity model default conditions



These materials have low water solubility, relatively high vapor pressure, and high log  $K_{ow}$ . These properties dictate that the material has a high potential to volatilize from water to air, but will adsorb to soil and sediments. When released to water part of the material will remain dissolved in water and will be removed through biodegradation and advection. A large amount will be released to air and be advected or reacted. When released to soil, the material will accumulate and then be removed through biodegradation and release to air where it will be advected or reacted. Since this material is susceptible to destructive reactions such as indirect photolysis and biodegradation, this material is expected to be short-lived in the environment (5-10 day residence times).

### 5. Bioaccumulation

A bioaccumulation study demonstrated a moderate potential of 1,4-diethylbenzene to bioconcentrate based on bioconcentration factors (BCF) of 320-629 in carp in 6 weeks at 25°C (MITI,1992; SIDS Dossier, 1994; SIDS SIAR, 1994).

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### C. Ecotoxicity

Aquatic toxicity endpoints for the OECD SIDS/HPV Chemical program include acute toxicity to freshwater fish, invertebrate, and alga. These endpoints have been determined (Hicks, 2003a,b,c) for the Diethylbenzene Blend prepared from equal volumes of diethylbenzene samples provided by BP Amoco Chemical Company, The Dow Chemical Company and Sterling Chemicals, Inc.

In an acute toxicity study (static-renewal system) with Rainbow Trout (*Oncorhynchus mykiss*), the tested Diethylbenzene Blend resulted in a 96- hr LC<sub>50</sub> of 0.673 mg a.i./L. The 96-hr NOEC was estimated to be < 0.308 mg a.i./L (Hicks, 2002a). The acute toxicity of the Diethylbenzene Blend to the Water Flea (*Daphnia magna*) under a static-renewal system was also determined (Hicks, 2002b). The 24-hr EC<sub>50</sub> was estimated to be > 2.70 mg a.i./L and the 48-hr EC<sub>50</sub> was calculated to be 2.01 mg a.i./L. The 48-hr NOEC was 1.07 mg ai/L based on the lack of sublethal effects at all lower test concentrations (Hicks, 2002b). The toxicity of the Diethylbenzene Blend to the unicellular Green Alga (*Selenastrum capricornutum*) was also determined (Hicks 2003c). Based on area under the curve, the 72-hr E<sub>b</sub>C<sub>50</sub> for the Diethylbenzene Blend was 1.00 mg a.i./L. The 72-hr NOEC was 0.547 mg a.i./L. Based on growth rate, the 72-hr E<sub>r</sub>C<sub>50</sub> for the Diethylbenzene Blend was 1.21 mg a.i./L. the 72-hr NOEC was 0.547 mg a.i./L (Hicks 2003c). (Table 8)

**Table 8. Ecotoxicity Data for Diethylbenzene Blend**

Endpoint	Toxicity Value
Acute Fish Toxicity ( <i>O. mykiss</i> )	96 hr LC <sub>50</sub> = 0.673 mg a.i./L
Acute Invertebrate Toxicity ( <i>Daphnia sp.</i> )	48 hr EC <sub>50</sub> = 2.01 mg a.i./L
Alga toxicity ( <i>Psuedokirchneriella subcapitata</i> ) - Growth - Biomass	72 hr EC <sub>50</sub> = 1.21mg a.i./L 72 hr EC <sub>50</sub> =1.00 mg a.i./L

In previous studies, Mixed Diethylbenzenes has been shown to be slightly toxic to fish, daphnids, and algae (Tucker et al, 1987a,b; Ward et al., 1996a,b,c). However, the methods used in these studies are considered to be less than adequate for volatile test materials. 1,4-Diethylbenzene had also been tested in the OECD-SIDS Program and was

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shown to be moderately toxic to fish and daphnids, and slightly toxic to algae (EA, 1992; SIDS Dossier, 1994; SIDS SIAR, 1994). However, the documentation for these studies was considered less than adequate for robust summaries under the HPV Chemical Program.

### **D. Human Health Effects**

#### **1. Acute Toxicity**

Diethylbenzene-Rich Streams are characterized by low acute oral and dermal toxicity. Oral LD<sub>50</sub> of 2050 to 6900 mg/kg have been reported for Mixed Diethylbenzenes (Chevron, 1991a; Biodynamics, 1987a). In two studies with Mixed Diethylbenzenes, the dermal LD<sub>50</sub> was reported to be greater than 2000 mg/kg in rats (Chevron, 1991b) and greater than 5000 mg/kg in rabbits (Biodynamics, 1987b).

The oral LD50 for 1,4-diethylbenzene was greater than 2000 mg/kg in Sprague-Dawley rats (MHW, 1993a; SIDS Dossier, 1994; SIDS SIAR, 1994).

Mixed Diethylbenzenes caused reversible moderate skin irritation (average scores at 24, 48, and 72 hours were 3.1 for erythema and 0.4 for edema; Draize score of 3.4 of a possible 8.0 after a 4-hour exposure) (Chevron, 1990a) and slight to moderate conjunctival irritation (Draize score of 2.7 of a possible 110) (Chevron, 1990b). Mixed Diethylbenzenes tested by Monsanto (1992) caused similar eye and skin irritation. Mixed Diethylbenzenes were negative for skin sensitization potential (Chevron, 1991c).

#### **2. Subchronic Toxicity**

Rats were exposed by inhalation to Mixed Diethylbenzenes at 0, 190, 610 and 1400 mg/m<sup>3</sup> for 10 weeks, six hr/day, five days per week (Kaempfe and Thake, 1993). The NOAEL was 190 mg/m<sup>3</sup>. Mean body weights were observed in the high-dose group throughout the study. There were no treatment-related abnormal clinical observations or ocular abnormalities. Treatment-related changes in hematologic parameters included moderate decreases in total white cell and lymphocyte counts in the mid- and high-exposure level males. Abnormal sera color (blue or blue-gray) was observed in high-exposure level males and females. Treatment-related changes in serum chemistry parameters included decreases in alanine aminotransferase, aspartate aminotransferase and creatinine phosphokinase in high-exposure level females and increases in potassium in high-level males and phosphorus in males from the high-exposure group and females from the mid- and high-exposure groups. An abnormal blue-gray color was observed in most tissues from all but one high-exposure animal. At the mid-exposure level, the same color was observed in brains and in the urinary bladders of some animals. This abnormal color probably resulted from the presence of the parent chemical or a metabolite in these

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tissues. There were no other gross or macroscopic changes attributed to the test material, including no effects on reproductive organs of either sex.

Rats given diethylbenzene (DEB) mixture with either 500 or 750 mg/kg exhibited a blue discoloration of the skin and urine as soon as the 3<sup>rd</sup> day of treatment. A significant reduction in weight gain was observed from the first week of treatment in the group treated with 750 mg/kg. Two animals died in the 750 mg/kg dose group during the first week of treatment. Two rats died in the 500 mg/kg group during the 4<sup>th</sup> and 7<sup>th</sup> weeks of treatment. No animals died in the control group. Rats in the DEB-dosed groups developed severe weakness in hind limbs and disturbances in gait from the 4<sup>th</sup> week of treatment. This weakness got worse in the following weeks, resulting in a complete paralysis of the hind limbs for some rats. There was a time-dependent decrease in MCV, SCV, and ASAP.

### 3. Neurotoxicity

Subchronic oral studies of Mixed Diethylbenzenes and diethylbenzene isomers, which focused on neurotoxicity, have been conducted (Gagnaire et al., 1990). Mixed Diethylbenzenes were administered at 0, 500 or 750 mg/kg/day for 10 weeks, 5 days/week. In both treated groups, rats exhibited a blue discoloration of the skin and urine and two animals in each group died during the study. A significant reduction in body weight gain was observed from the first week in the high-dose group. Rats in the treated groups developed severe weakness in hind limbs and disturbances in gait that resulted in a complete paralysis of the hind limbs for some rats. There was a time-dependent decrease in motor conduction velocity, sensory conduction velocity and amplitude of the sensory action potential. The LOAEL was 500 mg/kg.

In the studies of the isomers, 1,2-diethylbenzene was administered at 100 mg/kg/day, 4 days/week for 8 weeks, whereas 1,3-diethylbenzene and 1,4-diethylbenzene were each administered at 500 mg/kg/day to rats for five days/week for 8 weeks (Gagnaire et al., 1990). There was an eight-week post-exposure observation period for the isomer studies. Rats given 1,2-diethylbenzene developed the same symptoms (decreased body weight, blue discoloration of the skin and urine, weakness of hind limbs, paralysis) as those described for the diethylbenzene mixture. Two rats died during the study. 1,3-Diethylbenzene and 1,4-diethylbenzene-treated rats did not display any signs of neurotoxicity or any other signs of systemic toxicity. During the recovery period, the 1,2-diethylbenzene treated rats regained weight and became more mobile, but presented trailing hind limbs when attempting to walk. On the 4<sup>th</sup> week of recovery, all animals treated with 1,2-diethylbenzene succeeded in standing up. A time-dependent decrease in motor conduction velocity, sensory conduction velocity and amplitude of the sensory action potential was observed in animals dosed with 1,2-diethylbenzene but not with 1,3- or 1,4-diethylbenzene. The LOAEL for 1,2-diethylbenzene was 100 mg/kg whereas the NOAEL was 500 mg/kg for 1,3- and 1,4-diethylbenzene.

In additional neurotoxicity evaluations, rats were exposed to a commercial mixture of diethylbenzene isomers by inhalation at approximately 500, 600, 700, 800 or 900 ppm for 6 hrs/day, 5 days/week, for 18 weeks (Gagnaire et al., 1992a). There were treatment-

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related weakness or paralysis of the hindlimbs and disturbance of gait (not observed at 500 ppm), changes in motor and sensory nerve conduction velocities, changes in amplitude of the sensory action potential, and/or changes in parameters of the brainstem auditory evoked potential. Thus, in these studies, diethylbenzene was neurotoxic following repeated exposure to high levels. Rats exhibited a blue discoloration of tissues and urine. A NOEL was not determined, but the lack of clinical signs at 500 ppm indicates a decreased response at that exposure level.

When administered by ip injection 4 days/week at 10 mg/kg for 11 weeks or at 2 mg/kg for 6 weeks, the metabolite 1,2-diacetylbenzene caused hindlimb weakness at 10 mg/kg, hindlimb weakness and disturbance in gait at 20 mg/kg, and a decrease in mean sensory and motor conduction velocities at both dose levels (Gagnaire et al., 1991).

In another study, 1,2-diethylbenzene administered orally at 75 and 100 mg/kg/day, 4 days/week for 8 weeks, and intraperitoneal injection of 1,2-diacetylbenzene at 10 or 15 mg/kg/day, 4 days/week for 8 weeks, produced time- and dose-dependent alteration in brainstem auditory evoked potentials which did not completely recover during an 8 or 10 week recovery period (Gagnaire et al., 1992b).

### 4. Genetic Toxicity

Mixed Diethylbenzenes was negative for the reverse mutation assay with *Salmonella typhimurium* strains TA98, TA100, TA1535, and TA 1537 with and without S-9 activation (Chevron, 1991d; Stankowski, 1988), and with *E. coli* WP2 uvrA with and without S-9 activation (Chevron, 1991d). Mixed Diethylbenzenes was also negative in an *in vivo* micronucleus study in which mice were dosed intraperitoneally with 1000, 2000, or 4000 mg/kg (Chevron, 1991e). In a chromosomal aberration study using Chinese hamster ovary cells, Mixed Diethylbenzenes was negative with and without S-9 activation (Myers and Fahey, 1989).

1,4-Diethylbenzene was also negative in a bacterial reverse mutation assay (*Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *E. coli* uvrA with and without metabolic activation) (MHW, 1993b; SIDS Dossier, 1994; SIDS SIAR, 1994). It was also negative in a Chinese hamster CHL cytogenetics assay with and without metabolic activation (MHW, 1993b; SIDS Dossier, 1994; SIDS SIAR, 1994).

### 5. Developmental Toxicity

Mixed Diethylbenzenes administered orally to pregnant rats on gestation days 6-16 at 20, 100 and 200 mg/kg did not cause birth defects or developmental variations (Mercieca, 1992). The NOEL for maternal toxicity (reduced body weights and food consumption) was 20 mg/kg, whereas the NOEL for fetal body weight effects was 100 mg/kg. Mixed Diethylbenzenes streams were not teratogenic in this study.

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1,2-Diethylbenzene was administered orally to pregnant Sprague-Dawley rats at 0 (corn oil vehicle), 5, 15, 25 and 35 mg/kg on gestation days 5-20 (Saillenfait et al., 1999). Maternal weight gain and food consumption were decreased in the rats that received 15, 25 and 35 mg/kg. There was no effect on number of live fetuses, implantations, non-surviving implantations per litter, or fetal sex ratios. Fetal body weights were reduced in a dose-related fashion in the groups receiving 15, 25 and 35 mg/kg. The NOEL for both maternal and fetal toxicity was 5 mg/kg. There was no treatment-related effect on external visceral and skeletal malformations. 1,2-Diethylbenzene was not teratogenic in this study.

### **6. Reproductive Toxicity**

In the subchronic inhalation study reported by Kaempfe and Thake, 1993 (see above), rats exposed by inhalation to Diethylbenzene-Rich Streams at 0, 190, 610 and 1400 mg/m<sup>3</sup> for 10 weeks, six hr/day, five days per week had no effects on reproductive organs of either sex.

Sprague-Dawley rats were dosed orally with 1,4-diethylbenzene at 0, 30, 150 or 750 mg/kg/day in the combined repeat dose and reproductive/developmental toxicity screen level (MHW, 1993a; SIDS Dossier, 1994; SIDS SIAR, 1994). Males were dosed for 44 days, including 14 days before mating and females from 14 days before mating until Day 3 of lactation. There were no effects on mating, fertility, estrus cycle, pup body weight, or gross abnormalities at any dose. A slight increase in duration of gestation and a slight decrease in viability index at Day 4 in male pups in the 750 mg/kg/day group were not considered treatment-related by the investigators.

Based on the lack of effects on reproductive organs in the subchronic inhalation study (Kaempfe and Thake, 1993) and the availability of the developmental study (Mercieca, 1992) as well as the reproduction screen with 1,4-diethylbenzene, there is sufficient information on reproduction endpoints for the HPV program.

### **7. Toxicokinetics**

In pregnant Sprague-Dawley rats given a single oral dose of 25 mg/kg, [<sup>14</sup>C] 1,2-diethylbenzene concentrations in the fetus measured at 28-60% of the levels in maternal plasma within the first 48 hours after dosing and were consistently lower than levels in the placenta (Saillenfait et al., 1999). Placental and fetal tissues accounted for < 0.35% of the administered dose. Thus, there was limited placental transfer to the developing rat fetus.

Gagnaire et al. (1991) reported 1,2-diacetylbenzene in urine from rats given 165 mg/kg 1,2-diethylbenzene orally on four consecutive days. In male Sprague-Dawley rats administered [<sup>14</sup>C] 1,2-diethylbenzene intravenously (1 mg/kg) or oral (1 or 100 mg/kg), radioactivity was rapidly absorbed and mainly excreted in the urine (65-76% of the dose), and to a lower extent in the feces (15-23% of the dose) or via exhaled air (3-5% of the

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dose) (Payan et al., 1999). Biliary metabolites were extensively reabsorbed from the gut and ultimately excreted in urine. The two main metabolites were two glucuronide conjugates, probably of the two enantiomers of 1-(2'-ethylphenyl) ethanol, suggesting that the main initial conversion step of the primary metabolic pathway appears to be the hydroxylation of the  $\alpha$ -carbon of the side chain. In this study, insignificant amounts of the neurotoxic metabolite 1,2-diacetylbenzene were detected in urine, bile and feces. Payan et al. (2001) reported that the two main metabolites of 1,2-diethylbenzenes in urine of treated rats are the glucuronide conjugates of two enantiomers of 1-(2'-ethylphenyl) ethanol. The metabolic steps, which lead to the conjugates, are under stereoselective control.

### **8. Carcinogenicity**

A study of the dermal carcinogenesis potential of diethylbenzene (composition not given) (10% in acetone) applied to the backs of C3H/HEJ mice found one squamous cell carcinoma whereas none were reported in control mice (BRRC, 1983). Historical control data were not presented.

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### APPENDIX 1: Summary of HPV Endpoints for Diethylbenzene -Rich Streams

HPV SIDS Endpoints	Test Material*	Data Summary	Reference
2.1 Melting Point	4	Freezing point is < -75 °C	Huntley, 2003b
2.2 Boiling Point	4	180.8 °C ± 1.7 °C	Huntley, 2003a
2.4 Vapor Pressure	4	210 ± 44 Pa at 10 °C 310 ± 35 Pa at 20 °C 530 ± 15 Pa at 30 °C	Huntley, 2003c
2.5 Partition Coefficient (Log Kow)	3	3.72 for 1,2-Diethylbenzene 3.44 for 1,3-Diethylbenzene 3.45 for 1,4-Diethylbenzene	HSDB, 2001
2.6.1 Water solubility	4	15.7 ± 1.4 mg/L in water	Haahn, 2003
<b>3.1 Stability</b>			
<b>a. Photodegradation</b>	3	Direct: No significant contribution to degradation.	Technical Discussion
	3	Indirect: Atmospheric half-life of 0.75 – 1.5 days.	QSAR/EPIWIN (Calculation)
<b>b. In Water</b>	3	No significant contribution to degradation.	Technical Discussion
<b>3.3.1 Transport between Environmental Compartments</b>	3	High potential to vaporize from water to air. Material will absorb to soil and sediments, but will be removed through biodegradation and release to air. Material will not persist in air	EQC Level I, II, & III Modeling and Technical Discussion
<b>3.4 Aerobic Biodegradation</b>	1	Not readily biodegradable. 4.7% after 28 days; 5.5% after 35 days Inherently biodegradable	Marks et al., 1995  EPIWIN (Calculated)
<b>3.6 Bioaccumulation</b>	3	Moderate potential of 1,4-diethylbenzene to bioconcentrate based on bioconcentration factors (BCF) of 320-629 in carp in 6 weeks at 25°C.	MITI,1992; SIDS Dossier, 1994; SIDS SIAR, 1994
<b>4.1 Acute Toxicity to Fish</b>	4	96 hr LC50 = 0.673 mg a.i./L ( <i>Oncorhynchus mykiss</i> )	Hicks, 2002a
<b>4.2 Acute Toxicity to Aquatic Invertebrates (Daphnid)</b>	4	48 hr EC50 = 2.01 mg a i./L ( <i>Daphnia magna</i> )	Hicks, 22002b
<b>4.3 Acute Toxicity to Aquatic Invertebrates (Algae)</b>	4	Growth: 72 hr EC50 = 1.21 mg a.i./L ( <i>Selenastrum capricornutum</i> ) Biomass: 72 hr EC50 = 1.00 mg a.i./L ( <i>Selenastrum capricornutum</i> )	Hicks, 2002c
<b>5.1.1 Acute Oral Toxicity</b>	1	(A) Rat LD <sub>50</sub> = 2050 mg/kg (both sexes) (B) Rat LD <sub>50</sub> = 6900 mg/kg (males) and 4700 mg/kg (females)	(A) Biodynamics, 1987 (B) Chevron, 1991a

## Report for The Diethylbenzene -Rich Streams HPV Category

### APPENDIX 1: Summary of HPV Endpoints for Diethylbenzene -Rich Streams (continued)

HPV SIDS Endpoints	Test Material*	Data Summary	Reference
5.1.3 Acute Dermal Toxicity	1	(A) Rabbit LD <sub>50</sub> = >5000 mg/kg (B) Rat LD <sub>50</sub> = >2000 mg/kg	(A) Biodynamics, 1987 (B) Chevron, 1991b
5.4 Repeated Dose Toxicity	1,2,3	(A) NOAEL = 190 mg/m <sup>3</sup> (B,C) Specialized neurotoxicity studies: Oral: LOAEL = 500 mg/kg/day Inhalation: LOAEL = 500 ppm	(A) Kaempfe and Thake, 1993 (B) Gagnaire et al., 1990 (C) Gagnaire et al., 1992a
5.5 Genetic Toxicity <i>In Vitro</i>	1	(A, B) Negative for bacterial mutations (C) Negative for chromosomal aberration in Chinese hamster ovary cells	(A) Chevron et al., 1991a (B) Stankowski, 1988 (C) Myers and Fahey, 1989
5.6 Genetic Toxicity <i>In Vivo</i>	1	Negative for micronuclei in bone marrow erythrocytes	Chevron, 1991e
5.8 Reproductive Toxicity	1,3	(A) No effect on reproductive organs in subchronic study (B) Reproduction screen with 1,4-diethylbenzene. NOAEL = 750 mg/kg/day	(A) Kaempfe and Thake, 1993 (B) MHW, 1993a; SIDS Dossier, 1994; SIDS SIAR, 1994
5.9 Developmental Toxicity	1,3	(A) Rat oral gavage with Mixed Diethylbenzenes Maternal NOAEL = 20 mg/kg/day Developmental NOAEL = 100 mg/kg/day (B) Rat oral gavage with 1,2-DEB Maternal NOAEL = 5 mg/kg/day Developmental NOAEL = 5 mg/kg/day	(A) Mercieca, 1992 (B) Saillenfait et al., 1999

\*Test Material code:

1 = Mixed Diethylbenzene Stream (CAS No. 25340-17-4)

2 = Diethylbenzene isomers (mixed)

3 = 1,2- or 1,3- or 1,4-diethylbenzene

4 = Diethylbenzene Blend (Equal portions of 3 commercial producers' product)

## Report for The Diethylbenzene -Rich Streams HPV Category

### APPENDIX 2

Please note that the Polyethylbenzene Bottoms (CAS Registry #68987-42-8: benzene, ethylated, residues) is being tested separately under the HPV Chemical Program. The composition of Polyethylbenzene Bottoms listed below is based on capillary GC analysis of samples submitted by the eight participating companies to BP Amoco Analytical Technology (BP Amoco, 2000).

<b>Composition</b>	<b>Wt%</b>
Diphenylethanes	15 – 32
Diphenylmethanes	1 – 31
Other diphenylalkanes	7 - 12
Ethyl diphenylethanes & diethylbiphenyls	10 - 21
Polyethylbenzenes	<0.1 - 19
Triethylbenzenes	<1 – 26
Diethylbenzenes (m-, o-, p-)	<0.5
Butylbenzenes	<0.1
Other alkylbenzenes	9 – 24
PNAs (3-ring)	0.4 – 11
Ethylbenzene	<0.1
Benzene	<0.1
Paraffins/Naphthenes	<0.3
Total of unidentified components each present at <0.1%	3 – 6