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The QTRACER Program for Tracer-Breakthrough Curve Analysis for Karst and Fractured-Rock Aquifers

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PREFACE

The National Center for Environmental Assessment (NCEA) has prepared this document for the benefit of EPA regional offices, States, and the general public because of the need to develop a fast and easy method for evaluating tracer-breakthrough curves generated from tracing studies conducted in karst and fractured-rock aquifers. Results may then be applied in solute-transport modeling and risk assessment studies.

The purpose of this document is to serve as a technical guide to various groups who must address potential and/or existing ground-water contamination problems in karst and fractured-rock terranes. Tracing studies are always appropriate and probably necessary, but analyses can be difficult and tedious. This document and associated computer programs alleviate some of these problems.

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The National Center for Environmental Assessment within the U.S. Environmental Protection Agency's Office of Research and Development was responsible for the preparation of this document and provided overall direction and coordination during the production effort.

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ABSTRACT

Tracer tests are generally regarded as being the most reliable and efficient means of gathering subsurface hydraulic information. This is true for all types of aquifers, but especially so for karst and fractured-rock aquifers. Qualitative tracing tests have been conventionally employed in most karst sites in the United States. Quantitative tracing tests are employed sparingly at karst sites in the United States, although it is widely recognized that they provide a wealth of hydraulic and geometric data on subsurface conditions. Quantitative tracer tests are regarded as more difficult and time-consuming than qualitative tracing tests, which is a fallacy to be overcome. The benefits of quantitative tracing far outweigh any additional expenses that are incurred.

An efficient, reliable, and easy-to-use computer program, QTRACER, designed to run on PCs running any version of MS-DOS® or Windows®, has been developed to facilitate tracer-breakthrough curve analysis. It solves the necessary equations from user-generated data input files using robust integration routines and by relying on established hydraulic models. Additional features include dynamical memory allocation, ability to extrapolate late-time data using any one of three different methods, two separate methods for handling oversized time-concentration data files, and a powerful interactive graphics routine.

Two other programs are included to facilitate the use of QTRACER. The first, NDATA, allows the user to interpolate either their time-concentration or time-discharge data files to fill in data gaps. The second program, AUTOTIME, allows the user to convert time-concentration data files recorded using military time into sequential decimal time as required by QTRACER. Files created by these two programs may be appended to the bottom of a sampling station data file that can be read by QTRACER.

1. INTRODUCTION

Quantitative tracing studies in karst and fractured-rock aquifers are ground-water tracing studies designed to provide detailed information regarding the subsurface-flow dynamics of the aquifers. Such flow-dynamics information generally cannot be obtained from qualitative ground-water tracing studies, although some aspects are often inferred (Smart et al., 1986). Quantitative tracing studies consist of nothing more than the development of a tracer budget, *i.e.*, comparing the amount of tracer injected into the aquifer system with the amount of tracer recovered over time in conjunction with ground-water discharge measurements.

1.1. LIMITATIONS OF THIS REPORT

Although this report is intended to be generic in terms of tracer materials used, much of the report will focus on the use of fluorescent tracer dyes because of their inherent desirabilities (Field et al., 1995). Field and Mushrush (1994) also established the value of tracing petroleum contaminated ground water using the common tracer dye fluorescein. The numerical methods described herein and the accompanying computer programs are not tracer specific and thus may be used with any type of tracer material, provided it does not degrade or decay. For example, the analyses described do not account for the specific radioactive decay that will occur with radioactive tracers.

Additionally, most of this report will focus on tracing karst aquifers to define environmental problems. Karst aquifers are commonly considered to be the types of aquifers most in need of tracing studies. Many professional hydrologists are beginning to realize that fractured-rock aquifers are just as much in need of tracing studies as are karst aquifers, but in general tracing fractured-rock aquifers still receives minimal acceptance.

Many aspects of quantitative tracing studies are no different than those of qualitative tracing studies. The main difference is the level of information desired. As a consequence, the reader is referred to the work by Gaspar (1987a,b) and Mull et al. (1988) for good discussions regarding tracer tests in karst and fractured-rock terranes. Readers must decide for themselves if a qualitative tracing test is all they need or if a quantitative tracing test will better meet their needs.

In those instances where field techniques applicable to quantitative tracing vary from those applicable to qualitative tracing, an appropriate discussion will ensue. The reader may want to note that the major difference between quantitative and qualitative tracing

studies is mostly one of mathematical analysis and interpretation based on a more comprehensive tracer-sampling program.

1.2. PURPOSE

A decision to conduct quantitative tracing studies is based primarily on the need to know specific attributes of the aquifer being studied or monitored. For example, because of the complexity of ground-water flow in karst and fractured-rock aquifers, ground-water monitoring can be very difficult. The main purposes of this document is to illustrate the advantages of conducting quantitative tracing tests and to introduce the computer program, QTRACER for tracer-breakthrough curve analysis.

QTRACER is an efficient, reliable, and easy-to-use computer program designed to run on PCs running any version of MS-DOS® or Windows®. It was developed to facilitate tracer-breakthrough curve analysis. QTRACER solves the necessary equations from user-generated data input files using robust integration routines and by relying on established hydraulic models. Additional features include dynamical memory allocation, ability to extrapolate late-time data using any one of three different methods, two separate methods for handling oversized time-concentration data files, and a powerful interactive graphics routine.

1.2.1. Quantitative Tracer Tests to Support Ground-Water Monitoring Efforts

Qualitative ground-water tracing may establish a positive connection between a contamination source (Figure 1) and the monitoring locations, but probably will not provide sufficient evidence as to whether or how much leachate may be escaping past the monitoring points. Quantitative ground-water tracing provides a measure for determining the effectiveness of the monitoring system by estimating the tracer loss involved. Inadequate tracer recoveries are an indication that losses other than sorption or decay (*e.g.*, tracer migration to unmonitored locations) may be significant.

1.2.2. Quantitative Tracer Tests for Risk Assessments

When dealing with hazardous waste sites (*e.g.*, Superfund sites), proof of the adequacy of the existing or slightly modified ground-water monitoring system may be insufficient when evaluating the risk posed by the site. A site risk analysis requires a complete description of the release of the risk agent, its fate and transport in ground water and/or the epikarstic

Figure 1. Contaminant leakage from a pesticide storage warehouse into a sinkhole located in Manati, Puerto Rico. Pollutant stream is yellow color and black sludge is buildup from past releases.

zone, and any associated human and ecological exposure. To this end, it is necessary that all contaminant source areas and types of sources be identified, that actual time of travel of contaminants to all downgradient receptors be established, and that downgradient concentrations be properly quantified. Quantitative tracing studies are an essential part of any risk assessment of hazardous sites located in karst and fractured-rock terranes because such studies provide much of the necessary information that otherwise could not be obtained (Field and Nash, 1997; Field, 1997).

1.2.3. Quantitative Tracer Tests for Solute-Transport Parameter Estimation

In other instances it may be desirable to model the aquifer system using theoretically based solute-transport models. To calibrate these models to run in the direct mode (time-concentration estimates), good parameter estimates are essential. Hydraulic and geometric parameter estimates are most reliably obtained from tracer tests (Field and Nash, 1997). Theoretically based models run in the inverse mode (parameter optimization) can and should be used to calibrate the parameters estimated from quantitative tracer tests prior to evaluating contaminant migration by modeling solute transport in the direct mode (Małoszewski, *pers. comm.*).

Field (1997) used parameters estimated from a quantitative tracing test in a solute-transport model (TOXI5) to effectively calibrate the model for use in estimating the fate and transport of a hypothetical release of ethyl benzene. The model was run in the direct mode to produce estimated ethyl benzene concentrations at a downgradient spring used for drinking water.

Field et al. (1998) used a theoretical two-region nonequilibrium model to optimize parameters estimated from a series of tracer tests to demonstrate the effect of immobile flow zones (dead zones) on solute migration. Parameter estimation using the advection-dispersion equation, the two-region model, or even a three-region model requires that reasonably reliable parameter estimates be employed so that a global minimum can be found during optimization.

1.3. QUALITATIVE VERSUS QUANTITATIVE TRACING

Many well-head protection studies and landfill investigations/monitoring may be adequately addressed by qualitative tracing studies. Recharge/discharge areas are routinely established from successful qualitative dye-tracing studies and are commonly used to establish simple classes of conduit networks (Atkinson et al., 1973; Brown, 1973; Smart, 1988a).

Qualitative dye-tracing studies are often used to estimate apparent pollutant transport rates from apparent tracer velocities. Given the potential for additional costs and labor associated with conducting and interpreting quantitative tracing studies, qualitative tracing studies are often considered appropriate, but this may not be true. In other instances, however, additional details of the aquifer under investigation need to be established.

It has been suggested that quantitative tracing studies are too expensive because of (1) required sampling at a frequency sufficient to yield reliable results and (2) there are too many possible places the tracer might go, which would require frequent sample collection at tens or even hundreds of locations. Neither of these two items are valid, however.

With the advent of low-cost programmable automatic water samplers, continuous flow-through filter fluorometers (Figure 2), and recently developed fiber-optic fluorometers (Barczewski and Marshall, 1992; Benischke and Leitner, 1992) and spectrophotometers, adequate sampling frequencies are easily established. The only difficulty is the necessary power options, but automatic water samplers do not draw very much power and can be run on battery power for long periods.

Quantitative tracing studies have proved that a generalized estimate for ground-water flow directions based on potentiometric-surface maps, geological structure, and geological stratigraphy can be developed. Therefore, tracing experts can provide a reasonably good guess where tracers may be recovered without having to sample "everywhere," as has been advocated in the past. In addition, a "...well-designed tracer test, properly conducted, and correctly interpreted..." (paraphrased from James F. Quinlan) is likely to provide sufficient information for a determination as to whether tracer migration to unmonitored locations has occurred.

Quantitative tracing studies can be more valuable than qualitative tracing studies for answering specific questions, although quantitative tracing studies are often conducted after qualitative tracing studies have adequately established the ground-water flow trajectories and apparent ground-water flow velocities so that costs and labor efforts may be minimized. Ground-water problems, such as pollution migration from hazardous waste landfills, often demand more sophisticated quantitative ground-water tracing studies because of the need to better define subsurface hydraulic processes. They can also provide significantly more and better insights into the functioning of the aquifer than can qualitative tracing studies. Reliable estimates for tracer mass recovery, mean residence times, mean ground-water flow velocities, longitudinal dispersion, and maximum volume of aquifer conduits allow for useful evaluations of the hydraulic processes of dispersion, divergence, convergence, dilution, and

Figure 2. A Turner Designs® Model 10AU field filter fluorometer operating in the flow-through mode at Pearl Harbor Naval Base. Red valve is set horizontal to allow inflow of water from the bottom connector and discharge out the top connector.

storage (Atkinson et al. 1973; Smart, 1988a; Field and Nash, 1997). Such improvements in karst aquifer evaluation efforts translate into better ground-water resource management, ground-water monitoring designs, and ground-water remediation (Smart, 1985).

Finally it must be noted that qualitative tracing studies can lead to serious misinterpretations regarding aquifer connections. Smart et al. (1986) compared the results of qualitative and quantitative tracing for the Traligill Basin in Scotland and determined that the qualitative tracing results did not properly establish the subsurface connections.

2. TRACER TEST DESIGN FACTORS

Conducting quantitative tracing studies requires considerable knowledge of the tracer type employed, because simple measurement errors may occur as a result of tracer-specific effects, inappropriate sampling, and/or inappropriate analysis (Smart, 1988a). Smart and Laidlaw (1977) and other sections of this document discuss specific attributes of many of the fluorescent dyes commonly used for tracing ground-water flow. Field et al. (1995) provide a comprehensive discussion of the toxicity characteristics of several fluorescent dyes commonly used for tracing studies. Some typical fluorescent dyes used for tracing are listed in Table 1 and their structures shown in Figure 3.

Table 1. Some commonly used fluorescent dye types and their dye names with their respective Colour Index and CAS numbers.

Dye Type and Common Name	Colour Index Generic Name	CAS No.
Xanthenes		
sodium fluorescein	Acid Yellow 73	518-47-8
eosin	Acid Red 87	17372-87-1
Rhodamines		
Rhodamine B	Basic Violet 10	81-88-9
Rhodamine WT	Acid Red 388	37299-86-8
Sulpho Rhodamine G	Acid Red 50	5873-16-5
Sulpho Rhodamine B	Acid Red 52	3520-42-1
Stilbenes		
Tinopal CBS-X	Fluorescent Brightener 351	54351-85-8
Tinopal 5BM GX	Fluorescent Brightener 22	12224-01-0
Phorwite BBH Pure	Fluorescent Brightener 28	4404-43-7
Diphenyl Brilliant Flavine 7GFF	Direct Yellow 96	61725-08-4
Functionalized Polycyclic Aromatic Hydrocarbons		
Lissamine Flavine FF	Acid Yellow 7	2391-30-2
pyranine	Solvent Green 7	6358-69-6
amino G acid	—	86-65-7

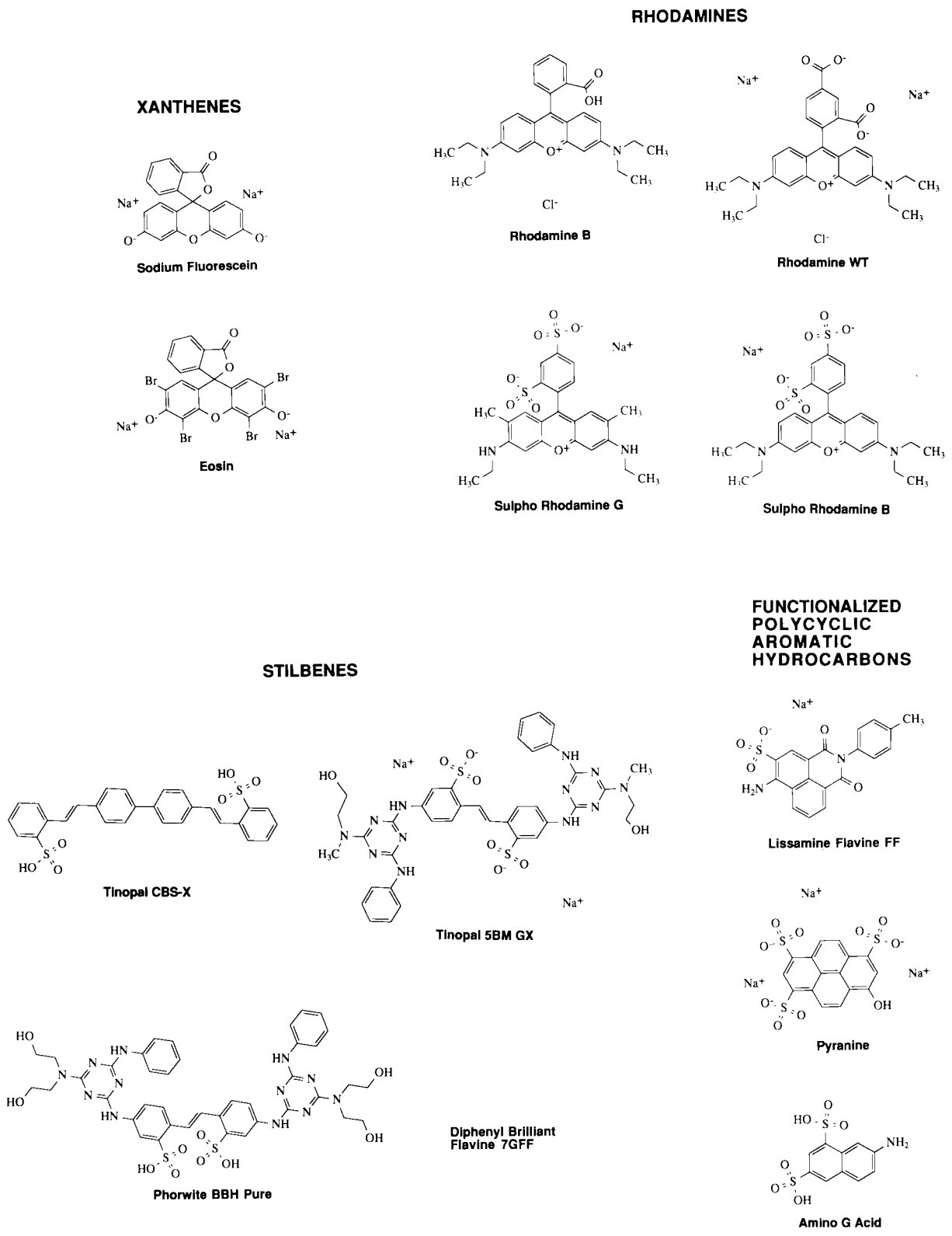

Figure 3. Chemical structures for selected fluorescent dyes used for water tracing.

Appropriate sampling efforts and frequencies for both tracer dye and ground-water discharge exert considerable influence on the accuracy of quantitative dye-tracing studies. Analytical methods must yield results with a high degree of precision as well. The fluorescent dyes listed in Table 1 fluoresce in the visible light spectrum anywhere from about 435 nm (Tinopal CBS-X) to approximately 584 nm (Sulpho Rhodamine B) (Table 2) (Figure 4).

Table 2. Data on some common fluorescent tracer dyes.

Dye Name	Maximum Excitation λ (nm)	Maximum Emission[1] λ (nm)	Fluorescence Intensity (%)	Detection Limit[2] (μg L^{-1})	Sorption Tendency
sodium fluorescein	492	513	100	0.002	very low
eosin	515	535	18	0.01	low
Rhodamine B	555	582	60	0.006	strong
Rhodamine WT	558	583	25	0.006	moderate
Sulpho Rhodamine G	535	555	14	0.005	moderate
Sulpho Rhodamine B	560	584	30	0.007	moderate
Tinopal CBS-X	355	435	60	0.01	moderate
Phorwite BBH Pure	349	439	2	?	?
Diphenyl Brilliant Flavine 7GFF	415	489	?	?	?
Lissamine Flavine FF	422	512	1.6	?	?
pyranine	460[3]	512	18	?	?
	407[4]	512	6	?	?
amino G acid	359	459	1.0	?	?
sodium napthionate	325	420	18	0.07	low

1. Values are approximate *only*. Different instruments will yield slightly different results.
2. Typical values for tracer detection in clean water using spectrofluorometric instrumentation.

Values may be adversely affected by augmented fluorescence and/or scattered light background.

Values will be lower when using filter fluorometric instrumentation.

3. pH ≥ 10
4. pH ≤ 4.5

Source: Behrens, 1986., Worthington, *pers. comm.*

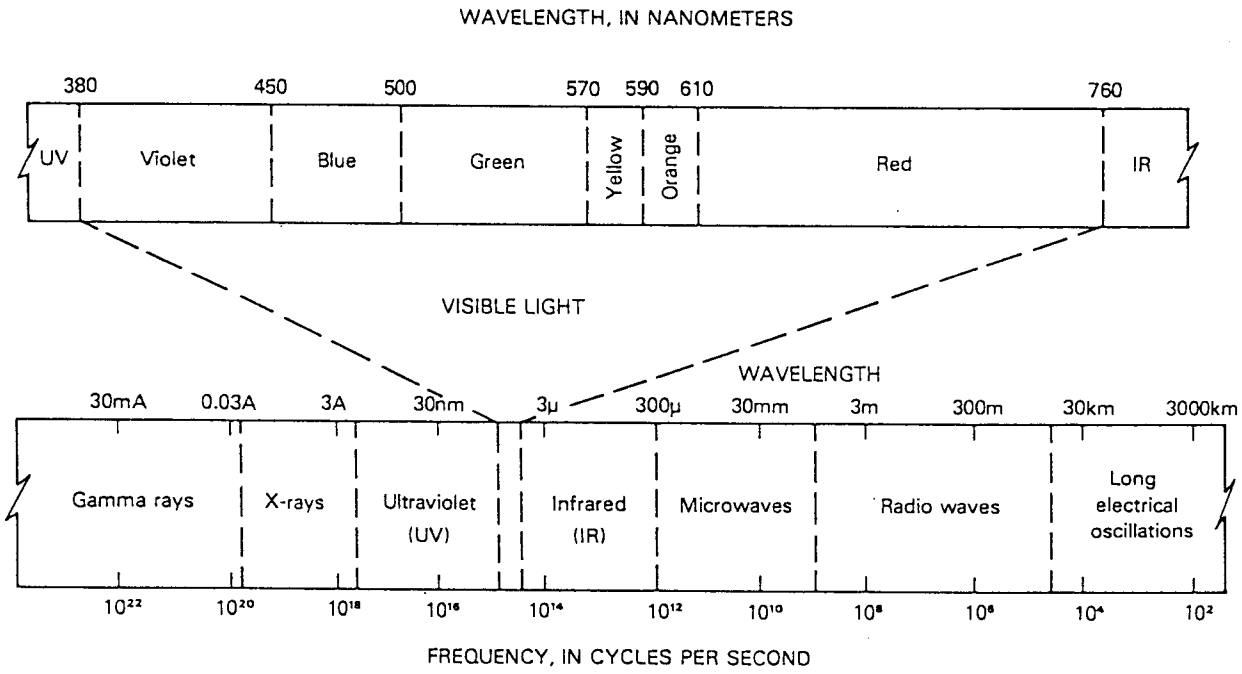

Figure 4. Electromagnetic spectrum with enlargement of visible spectrum for tracer dyes. Modified from Wilson et al. (1986, p. 3).

Lastly, different types of karst-conduit and fracture-flow networks will have a significant effect on tracer mass recovery, but such knowledge may be unknown to the tracing professional. These factors can be problematic when interpreting either qualitative or quantitative tracing study results and cannot be ignored.

2.1. TRACER CHARACTERISTICS

All chosen tracer substances should exhibit certain "ideal" characteristics, most notably conservative behavior. Unfortunately, no tracer substance is ideal, but fluorescent dyes are appropriate for tracing subsurface flow because of their low purchase cost, ease of use (injection, sampling, and analysis), low toxicity, relatively conservative behavior, high degree of accuracy of analysis, and low cost of analysis. However, specific aspects of any particular tracer dye chosen for a tracing study may adversely affect tracer recovery and thus lead to incorrectly calculated results (*e.g.*, mass-balance errors).

When conducting qualitative dye-tracing studies, it is usually sufficient to inject a known quantity of dye on an "as sold" basis which means that a considerable amount of diluent has been added to the dye (*i.e.*, $< 100\%$ dye). However, when conducting quantitative dye-tracing studies, the actual mass of dye injected into the aquifer must be known if the calculations are to be performed correctly.

Consider, for example, the commonly used fluorescent-tracer dye Rhodamine WT (Acid Red 388). For a qualitative trace, the tracing professional may decide to inject 18 pounds (2 gallons on an "as sold basis") into the aquifer and be satisfied with the outcome. A quantitative trace would, however, require that the actual mass of the dye injected be calculated because Rhodamine WT is sold as a 20% solution (actually it is sold as a 17.5% solution, but is listed as a 20% solution) and because it has a density of 1.16 g cm^{-3}. In this particular instance, the conversion to mass is developed from the following formula (Mull et al., 1988, p. 61):

$$V \times \rho \times \% = M_{in} \tag{1}$$

where V is volume [cm^3], ρ is density [g cm^{-3}], % is purity, and M_i is mass injected [g].

To determine the actual dye mass injected into the aquifer, the user must perform the following calculations:

1. Convert gallons to equivalent SI units (cubic centimeters for this example)

$$2.0 \text{ gal} \times 3.785 \times 10^{-3} = 7.570 \times 10^{3} \text{ cm}^3$$

where 3.785×10^{-3} is a conversion factor.

2. Next insert the value obtained in step 1 into Equation (1)

$$\begin{aligned} 7.570 \times 10^{3}\ \text{cm}^3 \times 1.16\ \text{g cm}^{-3} \times 1.75 \times 10^{-1} &= 1.54 \times 10^{3}\ \text{g} \\ &= 1.54\ \text{kg} \end{aligned}$$

Subsequent quantification calculations would then use 1.54 kg for the mass of dye injected into the aquifer. Similar calculations for other tracer types need to be made using tracer-specific information.

Tracer sampling also presents some difficulty, depending upon the behavior of the tracer. All tracers will exhibit some loss due to sorption onto aquifer materials, but other factors may also cause a loss of tracer mass in the samples. For example, a commonly used dye for ground-water tracing, sodium fluorescein (Acid Yellow 73), tends to photodecay so that excess exposure to sunlight may diminish total mass recovery. Rhodamine WT is temperature dependent and requires correction of field measurements to a standard temperature. Even worse, it has recently been shown that Rhodamine WT naturally degrades to carboxylic fluorescein, which may substantially interfere with analyses and interpretations if sodium fluorescein was also used during the study (Gareth Davies, *pers. comm.*). Pyranine (Solvent Green 7) is *p*H dependent, which requires careful buffering of the water samples prior to analysis (Smart and Laidlaw, 1977).

2.2. TRACER INJECTION

Ground-water and surface-water tracing both require labeling or "tagging" the flowing water with some identifying substance (*i.e., tracer*) for subsequent detection at some distant point. This can only be achieved by getting the tracer to mix with the water. For surface-water tracing, this is not difficult. However, labeling ground water with a tracer can be fairly involved.

Typically, for karst systems the tracer substance, usually a fluorescent dye, is injected directly into a sinkhole or sinking stream that is believed to be connected to the karst conduit system. Figure 5 depicts a reinforced sinkhole located at the RCA del Caribe Facility (Barceloneta, Puerto Rico) that was used for plant waste-water injection and for tracer injection. Although small in appearance, this is a substantial entry point for water and pollutants.

Figure 5. Reinforced sinkhole receiving plant waste water at the RCA del Caribe Facility. Waste water appears as clear water discharging from the rust colored pipe inside the sinkhole.

Figure 6. Dissolutionally enlarged fissure in limestone where most flow will occur. Precipitation of calcium carbonate in fractures appears as white and/or brown streaks.

Boreholes and wells are often used as injection points, but these are not as effective as sinkholes and sinking streams. Sinkholes and sinking streams are directly connected to the subsurface "plumbing" system of a karst aquifer. Boreholes and wells, in general, are rarely connected to the subsurface flow system.

Once injected, the tracer will move through the conduit system. Figure 6 depicts two fairly typical karst conduits that may exist in an area. From Figure 6 it is obvious that if the two conduits shown were at a depth of approximately 10–30 meters, it would be nearly impossible to detect them by any known geophysical means or to intersect them by a well. Monitoring wells are next to useless in this instance. However, a slug of tracer dye will use these conduits to migrate to a point where detection is possible.

2.2.1. Methods of Injection

Tracer injection can use a variety of methods. For example, it is not atypical to observe an injection in which a powder or liquid dye is injected ("dumped" and "introduced" are synonyms) directly into a sinkhole, sinking stream, or monitoring well. However, it is usually desirable to mix powder tracers with water prior to injection to prevent site contamination by air currents. The tracer/water mixture is then more easily poured into the injection point. Powder tracer mixing is most easily accomplished by adding a measured quantity of tracer into a large carboy (*e.g.*, 5 L) containing a small quantity of water (Figure 7).

After the preferred amount of tracer has been added to the carboy, more water is added to the mixture to bring the level up to about one-half to one-third full. The cap is then screwed down tightly and the carboy shaken vigorously to effect a thorough mixing. The carboy should be weighed before and after all additions and after injection so that a reasonably accurate estimate of tracer mass can be accomplished. The contents of the carboy are then easily released into the injection point (Figure 8).

Prior to tracer injection a substantial quantity of water (*e.g.*, 1000 gal.) should be released into the sinkhole or monitoring well (this is unnecessary for sinking streams). This "primer" of water helps to flush out the system of any debris and to lubricate the system. The tracer may then be added to the inflowing water. Alternatively, the water injection may be halted for tracer injection and then restarted after tracer injection.

A large quantity of chaser water (*e.g.*, 3000 gal.) is injected after tracer injection to help move the tracer along. Chase water helps to prevent the tracer getting stored in large dead-end pores and behind other obstructions. However, it is necessary in some instances (*e.g.*, monitoring wells) that care be taken not to raise the head excessively.

2.3. TRACER SAMPLING

Sampling for tracer must be performed in conjunction with discharge measurements for quantitative tracing because ground-water discharge and tracer-mass recovery are strongly interconnected. If discharge is not measured during the tracing study, but water samples are collected, then the tracing study may be considered semiquantitative. Sampling must also be of sufficient frequency so as to avoid the problem of aliasing (Smart, 1988a). Aliasing occurs when sampling frequencies are inadequate (*i.e.*, time intervals between individual sampling events are too far apart), which may cause certain aspects of tracer recovery to

Figure 7. Mixing fluorescein powder dye with water in a 5 L carboy. Fluorescein is a brick red color when a dry powder.

Figure 8. Injecting mixture of water and fluorescein dye into an injection well. Fluorescein has as a very dark red color when concentrated as shown here, but becomes a bright fluorescent green when diluted.

not be observed.

Additionally, cessation of sampling prior to complete recovery of the tracer mass may lead to an inadequate estimate of the aquifer characteristics desired. Field and Nash (1997) demonstrated the efficiency of numerical interpolation/extrapolation algorithms to fill gaps in the sampling data record.

2.4. SAMPLING EQUIPMENT

Mull et al. (1988, pp. 38–39) recommend that samples be collected by automatic samplers using glass sample bottles so as to minimize losses. Automatic samplers can be programmed to collect a water sample at appropriate sampling frequencies so that even midnight samples may be conveniently collected. Glass sample bottles are less likely to sorb the tracer than are plastic sample bottles, which may distort sample analysis results. Even if automatic samplers are not to be used, glass sample bottles are still appropriate for sample collection. The sample bottles need only be large enough to hold a maximum of approximately 32 mL of water in most instances.

Grab samples using appropriately sized test tubes with caps (*e.g.*, 25 mm $\times$ 150 mm) minimize handling. Samples should be stored tightly capped in a cool dark place. Shipping to the laboratory should be by cooler with an ice block enclosed.

Packets of activated charcoal may also need to be collected if fluorescent dyes are used as tracers. It is believed that activated charcoal will ensure dye recovery because the much lower dye concentrations found in water samples may not be detected in the water, or sampling frequencies may not have been adequate. The ability of activated charcoal to continue sorbing and concentrating fluorescent dye provides a sound means for determining fluorescent dye occurrence when water samples are ambiguous. However, at best activated charcoal will result in a qualitative tracing test only. More seriously, there is considerably more opportunity for sample contamination from handling. Still more serious is the recently considered problem of false positives and false negatives associated with activated charcoal packets.

2.5. SAMPLING LOCATIONS AND FREQUENCIES

Sampling locations and frequencies can be based on the results of qualitative dye-tracing studies so that appropriate sampling locations and frequencies may be determined in advance of conducting quantitative tracing studies. Preliminary qualitative tracing studies

may help ensure that proper sample collection will occur while minimizing expenses when quantitative tracing efforts are undertaken.

Should quantitative ground-water tracing efforts be initiated prior to qualitative tracing efforts, it is possible that too many or too few sampling locations will be utilized; the former drives up the cost while the latter results in incomplete tracer mass recovery. Sampling frequencies may also be inadequate, with the result being added costs (excessive number of samples collected) or inadequate tracer mass recovery (not enough samples collected often enough). Preliminary simple ground-water tracing studies can be useful for more difficult and complicated tracing studies. However, as previously discussed (Section 1.3.), recent studies have proven that with a basic understanding of the local hydrogeology and the use of automatic water sampling equipment, qualitative tracing efforts need not be conducted prior to quantitative tracing efforts.

2.6. TRACER MIXING IN THE CONDUIT

Complete lateral and vertical mixing of the tracer in a conduit or fracture(s) is considered ideal but not always possible. An acceptable mixing length is one in which the travel distance allows for nearly complete lateral mixing of the tracer and is considered to be an important factor in tracing surface-water flows (Kilpatrick and Cobb, 1985, pp. 2–3). Unfortunately, ground-water tracing in karst and fractured-rock aquifers does not always ensure that adequate lateral mixing will occur in karst conduits or fractures because tracing efforts are constrained to the limits of tracer-injection points as related to tracer-recovery points. Inadequate mixing may result in incorrect tracer-recovery calculations.

Mull et al. (1988, pp. 43–44) recommend that sampling during preliminary traces occur (at a minimum) at three places in the cross-section of spring and the tracer-breakthrough curves plotted for each sampling point in the cross-section. Complete lateral mixing is determined to have occurred when the areas under the tracer-breakthrough curves for each sampling location are the same regardless of curve shape or magnitude of the peaks; optimum results are obtained when mixing is about 95% complete (Figure 9) (Kilpatrick and Cobb, 1985, p. 3).

2.7. CORRECTION FOR BACKGROUND

All field measurements need to be corrected by subtracting background tracer concentrations from measured tracer concentrations. For example, sodium fluorescein is used to color automobile antifreeze. Because there are so many automobiles in existence and so many of

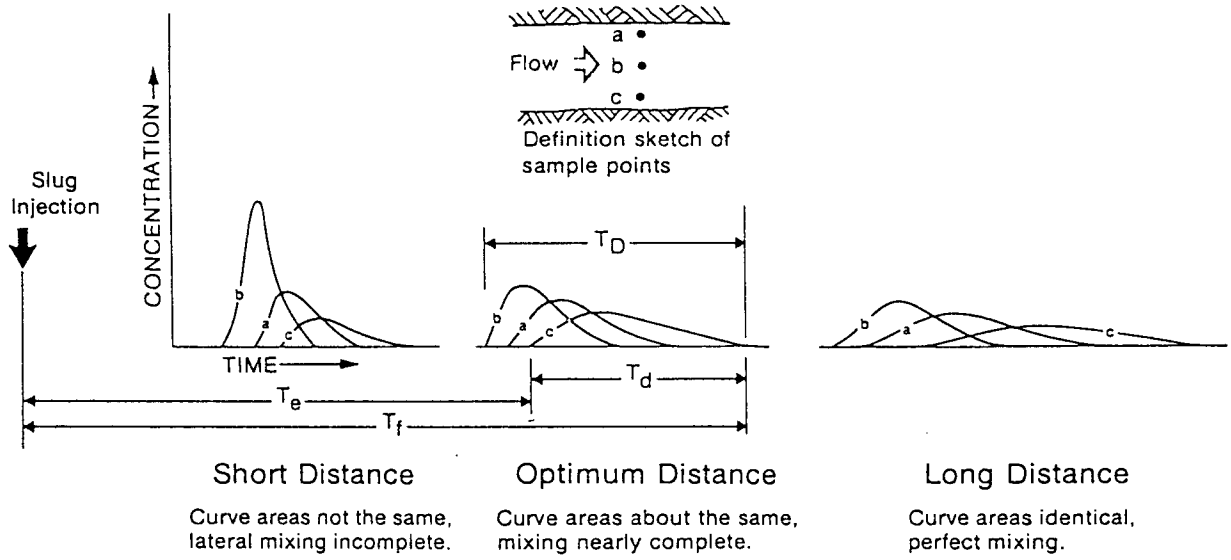

Figure 9. Typical response curves observed laterally and at different distances downstream from a slug injection of a tracer in the center of a stream (Kilpatrick and Cobb, 1985, p. 3).

them have leaks in their radiators, fluorescein-colored antifreeze is fairly ubiquitous in the environment.

Prior to any tracing efforts, background water samples need to be collected and analyzed for the tracer of interest. If the values obtained are low enough (*e.g.*, few μg L^{-1}), then the chosen tracer may be used; if not then a different tracer should be chosen. Low background concentrations in samples will then need to be averaged. This final value is then subtracted from every sample of recovered tracer from subsequent tracing efforts.

In addition, instrument calibration (*e.g.*, scanning spectrofluorophotometer and filter fluorometer) should be performed as described in the appropriate U.S. Geological Survey Techniques of Water-Resources Investigations publications (Kilpatrick and Cobb, 1985; Wilson et al., 1986). Proper instrument calibration is essential. Calibration using distilled water is common, but use of sample water is also acceptable.

2.8. DISCHARGE MEASUREMENTS

As stated previously, tracer sampling must be performed in conjunction with discharge measurements. If sampling is performed at wells that are being pumped at a constant rate, then discharge is fairly easily determined. Discharge at springs is considerably more difficult to estimate. If grab samples are being collected from nonpumping wells, then some estimate for flux past the well may need to be established.

Estimation of discharge may require special efforts on the part of the tracing professional. Weirs may need to be built, standpipes installed, flow meters utilized, and losses to evaporation estimated (for large bodies of water). Numerous documents describing methods for estimating discharge already exist, so the techniques will not be discussed here. Interested readers should examine the appropriate U.S. Geological Survey Techniques of Water-Resources Investigations publications for comprehensive discussion of discharge estimates.

Important to note is the possible occurrence of transient high-level overflows in which normally dry springs may discharge large quantities of water during storm events. Springs that are normally dry during low- to moderate-flow conditions may function during high-flow conditions. Efforts to address irregularly functioning springs should be prepared prior to initiating quantitative tracing studies so that discharge of tracer at such springs can be recovered.

Less common is the problem of sampling well screens set at elevations below which high-flow conditions occur. Such wells may be adequate for recovering tracer during low-

and moderate-flow conditions, but incapable of drawing in and discharging tracer during high-flow conditions. Presumably such an occurrence would be addressed by appropriate sampling at downgradient high-flow springs.

2.9. KARST CONDUIT NETWORKS

Tracing studies used in the determination of subsurface flow conditions in karst terranes are greatly influenced by various combinations of subsurface flow networks located between the inflow and outflow points of the aquifer. Seven types of karst networks are known to exist, as schematically shown on Figure 10.

The influence of karst networks on dye quantity present at a recovery site can be significant. If flow is through the simple Type I network, dye quantity estimates may be reasonably accurate. The more complex the karst network, however, the less likely it is that estimates of dye quantity will be adequate. As estimates become more difficult to make, it becomes tempting to use more dye than necessary. For Types II through VII (but excluding Type V), the estimate of dye quantity is likely to be low.

2.9.1. Network Types I, II, and III

If flow is through a Type I network, then predictions based on common tracing techniques may be reasonably accurate. If flow is through a Type II or Type III network, the accuracy of the predictions will tend to be inversely proportional to the amount of dye that is either diluted by additional water inflow or diverted to unknown discharge points. Distributary flow and multidirectional flow are subtypes of Types III and IV.

2.9.2. Network Types IV and V

Types IVa and IVb further complicate the flow determination because of significant loss of dye and because the identified outflow point will have a discharge rate that may be less than, greater than, or equal to the inflow point. Type V presents the worst situation related to flow prediction because no dye is recovered. This can lead to a false sense of a lack of hydraulic conductivity (*i.e.*, if the dye goes elsewhere, such results indicate there is no flow to the sites being monitored).

2.9.3. Network Types VI and VII

Types VI and VII are situations where either a significant amount of ground-water storage exists or a separate karst subsystem is connected to the main karst system. These are really

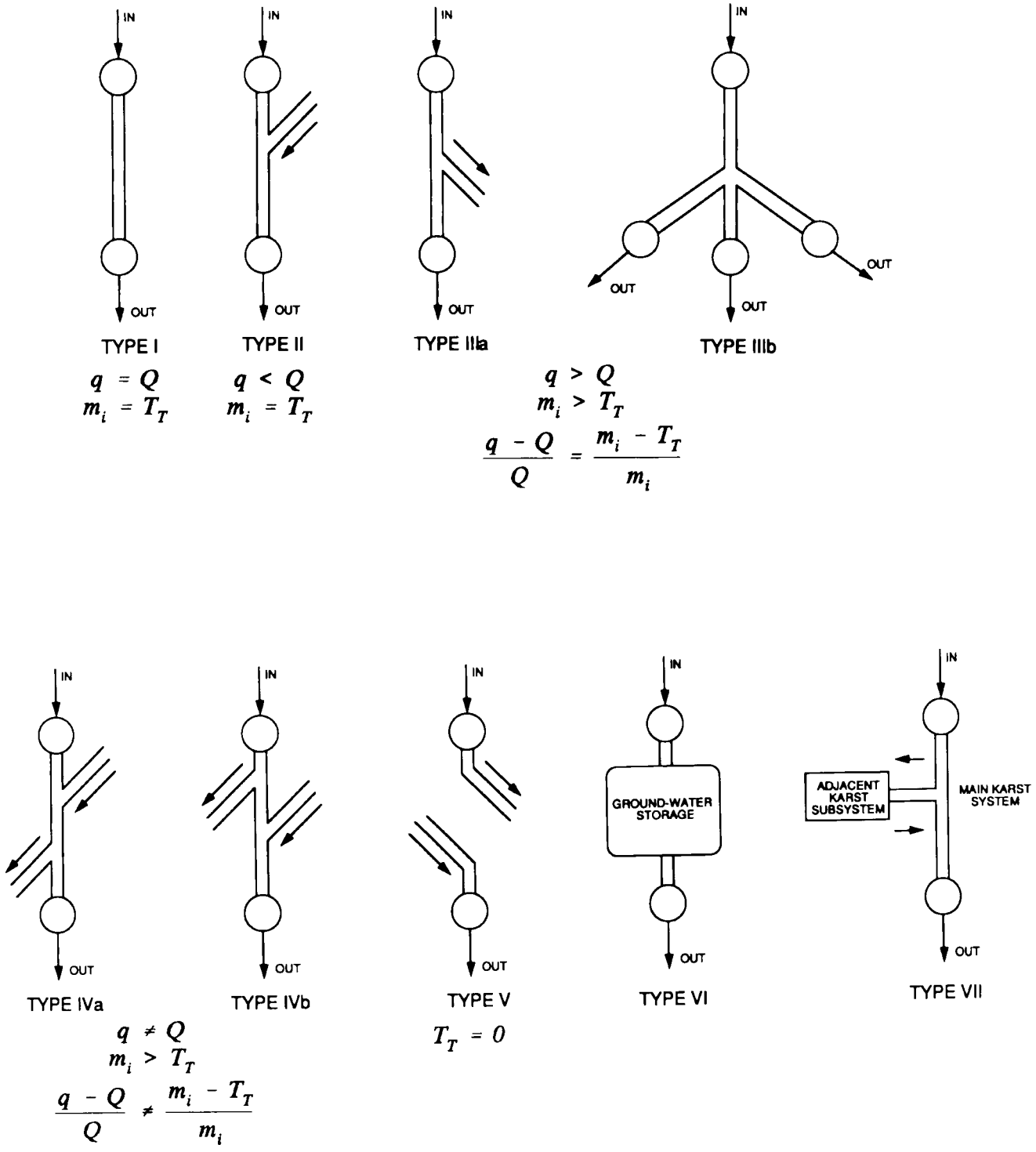

Figure 10. Seven simple karst network types that describe tracer migration in karst onduits. Any of there networks may significantly influence tracer tests between the point of inflow (IN) and the point of outflow (OUT) in a karst system. Discharge into the conduit is q, discharge out of the conduit is Q, tracer mass injected into the conduit is m_i, and tracer mass recovered is T_T. Note: Any one of these network types may be interconnected with any of the others. Modified from Atkinson et al. (1973) and Gaspar (1987b, p. 64).

subgroups of any one of Network Types I, II, III, IV, or V. As drawn, Network Types VI and VII appear only as subgroups of Network Type I, but additional inflows, outflows, or no connection to the sample-collection station(s) are realistic possibilities. For contaminant transport in a karst system, Network Types VI and VII may play significant roles.

2.10. DETERMINATION OF TOPOLOGICAL KARST CONDUIT NETWORK TYPE

Determination of the karst conduit network type usually requires extensive cave exploration, but can be roughly estimated from quantitative ground-water tracing studies. This is achieved by recognizing that each topological type exhibits specific characteristics that influence the results of tracing studies (Atkinson et al., 1973).

A Type I network (Figure 10) will exhibit such characteristics as inflow discharge equal to outflow discharge and mass of injected tracer equal to mass of recovered tracer

$$\begin{aligned} q &= Q \\ M_{in} &= M_{out} \end{aligned}$$

This assessment seems intuitively obvious considering that for both the inflow and outflow discharges to be equal and for complete tracer recovery to occur requires that a simple straight tube be defined. Other topological types become more difficult to assess as discharges and tracer recoveries become more complex (Figure 10).

It will be noted that Network Types VI and VII may fit into any one of the above categories, but with the added effect of storage in the system. Storage is not, however, accounted for in the simple relationships because it is only a delaying mechanism.

3. QUANTITATIVE TRACING METHODOLOGY

Quantitative tracing studies are based on a detailed study of tracer-breakthrough curves, which are generated from quantitative chemical analyses (*e.g.*, fluorescence) of a series of water samples in combination with ground-water discharge measurements for each sampling station at which tracer was recovered. Tracer-breakthrough curve shape for conduit-dominated karst aquifers depends upon:

- Character of the tracer.
- Prevailing flow conditions.
- Structure of the aquifer (Smart, 1988a) and similarly for fractured-rock aquifers.

Discussion of these conditions as related to tracer-breakthrough curves has already been addressed and also reviewed by Smart (1988a). Successful quantitative ground-water tracing studies are dependent upon:

- Conservative behavior of the tracer substance.
- Precise instrument calibration.
- Adequate quantity of tracer substance to be injected.
- Sufficient monitoring frequency at all downgradient receptors.
- Precise discharge measurements at downgradient receptors.
- Sufficient length of monitoring period for total tracer mass recovery.

These factors may be achieved through good design, implementation, and persistence.

Various problems tend to arise when the above factors are not considered in the design of a tracing study. Such problems may include no tracer recovery, incomplete tracer recovery, or aliasing of the tracer-breakthrough curve (Smart, 1988a). These problems lead to some fundamental questions regarding the tracing study. If none or only some of the injected tracer mass was recovered, what caused incomplete recovery? What was the mean residence time (mean tracer transit time) for the tracer in the aquifer? What were the mean and apparent tracer velocities assuming advection only? How significant was longitudinal dispersion in the aquifer?

In terms of contaminant transport, answers to these questions are essential. Some of the questions can only be answered by making best professional interpretations of the tracer-breakthrough curve. Others may be answered by careful numerical analysis of the tracer-breakthrough curve. For example, in instances of insufficient sampling frequency or cessation of sampling prior to total tracer mass recovery, good interpolation/extrapolation algorithms may be used to fill gaps in the data. However, problems of aliasing may not be addressed by such efforts while extrapolation of data beyond real sampling times may not provide realistic values.

3.1. ESTIMATION OF HYDRAULIC PARAMETERS

Hydraulic parameters for karst conduits and fractures are estimated by the method of moments. The zeroth moment is used to estimate the tracer mass recovery, the first moment is used to estimate the mean residence time and mean flow velocity, and the second moment is used to estimate the longitudinal dispersion. However, as will be shown, the second moment should not be relied upon for reliable estimates for dispersion.

Analysis by the method of moments is really nothing more than determining the area under the tracer-breakthrough curve generated by plotting time verses measured tracer concentrations (Figure 11).

The following discussion is taken from Kilpatrick and Wilson (1989, p. 3 and 4) because it is so eloquently stated and straightforward.

The tracer-breakthrough curves along a streamline shown in Figure 11 may be described in terms of elapsed time after a slug injection. Characteristics pertinent to the tracer-breakthrough curve analysis are

- T_L, elapsed time to the arrival of the leading edge of the tracer-breakthrough curve *at a sampling point.*
- T_p, elapsed time to the peak concentration C_p of the tracer-breakthrough curve *at a point.*
- T_c, elapsed time to the centroid of the tracer-breakthrough curve *at a point.*
- T_t, elapsed time to the trailing edge of the response curve *at a point.*

The mean travel time for the flow along a streamline is the difference in elapsed time of the centroids of the tracer-breakthrough curves defined upstream and downstream *on the*

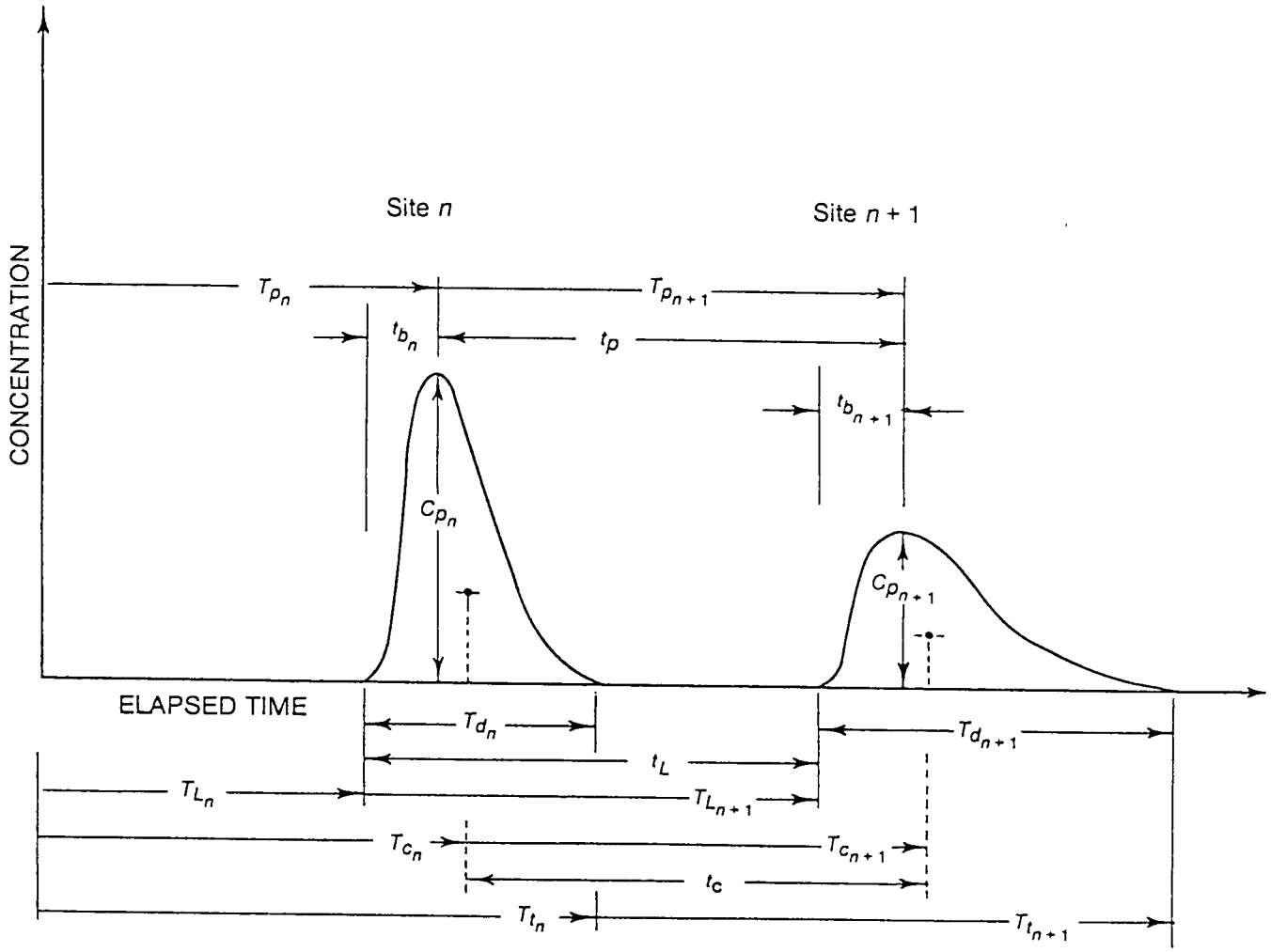

Figure 11. Definition sketch of tracer-breakthrough curves along a selected tracer streamline from an instantaneous tracer injection (Kilpatrick and Wilson, 1989, p. 3).

same streamline given by

$$t_c = T_{c_{(n+1)}} - T_{c_n} \tag{2}$$

where n is the number of the sampling site. Similarly, the travel times of the leading edge, peak concentration, and trailing edge *along a given streamline* are, respectively

$$t_L = T_{L_{(n+1)}} - T_{L_n} \tag{3}$$

$$t_p = T_{P_{(n+1)}} - T_{p_n} \tag{4}$$

and

$$t_t = T_{t_{n+1)}} - T_{t_n} \tag{5}$$

The time T_d necessary for the tracer mass to pass *a sampling point* in a section is

$$T_d = T_{t_n} - T_{L_n} \tag{6}$$

As shown in Figure 11, a typical tracer cloud may travel faster in the center of the stream than along the karst conduit or fracture walls, where it may also be more elongated. Complete definition of the tracer-breakthrough curve to a slug injection therefore may involve measurement at more than one point or streamline in several sections (if possible). Usually in karst and fractured-rock aquifer tracing, such elaborate sampling is not possible; samples are acquired where feasible. It also may not be necessary if adequate mixing has occurred. However, it is advisable to sample at least three points along a cross section of a spring to ensure adequate mixing.

The duration or time of passage of a tracer response *at a section* T_D is the difference between the slowest trailing time along a conduit or fracture wall and the fastest leading edge time, usually observed in the center. The difference between the values of T_d and T_D can be significant. It is usually assumed that $T_D \approx T_d$.

The remainder of this document will not rely on Equations (2)–(6) because it is rare for ground-water tracing studies to provide an opportunity to sample at multiple locations along a streamline. Direct access to a cave during a tracer test is one exception, however.

3.1.1. Total Tracer Recovery

Estimation of tracer recovery for individual sampling stations is given by Equation (7) (modified from Gaspar, 1987b, p. 62)

$$M_O = \int_0^\infty C(t)\, Q(t)\, dt \tag{7}$$

and total tracer recovery from all downgradient receptors may be estimated from Equation (8) (Gaspar, 1987b, p. 63)

$$M_T = \sum_{i=1}^{n} M_{O_i} \tag{8}$$

These models assume complete mixing of the tracer substance with water, negligible dispersion effects, and that the tracer mass will ultimately exit the aquifer system completely at one or more downgradient receptors as a function of time and discharge.

A simple total dye recovery equation for a single sampling station was developed by Mull et al. (1988, p. 52) that includes a necessary unit conversion factor because English and SI units are intermixed in their equation. Other than the necessary unit conversion factor, this equation yields acceptable results if proper care is taken in the execution of the tracing study. Their equation is not reproduced here to avoid confusion with Equation (7) of this section.

3.2. QUALITY OF TRACER MASS RECOVERY

The quality of the tracer experiment may be quantified in terms of mass recovered. Usually, the quality of the tracer experiment is given as percent of mass recovered, but this affords little insight. An accuracy index given by Sukhodolov et al. (1997)

$$A_I = \frac{M_{in} - M_T}{M_{in}} \tag{9}$$

provides more insight into the quality of the tracing experiment. An $A_I = 0$ indicates a perfect tracing experiment. A positive A_I indicates more mass injected than was recovered, while a negative A_I suggests more mass recovered than was injected. As A_I moves further away from zero, the quality of the tracing experiment gets poorer.

A high degree of precision for tracer recovery has considerable utility. For evaluation of ground-water monitoring and contaminant transport, total tracer mass recovery is essential. Tracer mass recovery should be quantified so as to ensure that all relevant locations are properly monitored for ground-water quality. Otherwise it is likely that important ground-water discharge locations may be missed. A low-percent recovery of a conservative tracer mass may be an indication of significant loss of tracer during the study, often a result of improper determination of downgradient receptors. A high-percent recovery is a probable indication that most if not all relevant downgradient receptors were properly monitored for tracer recovery. For contaminated sites of a controversial nature (*e.g.*, Superfund sites) this can be critical.

3.2.1. Mean Residence Time

Mean tracer residence time is the length of time required for the centroid (gravity mass) of the tracer mass to traverse the entire length of the aquifer system, representing the turnover time for the aquifer. The centroid is generally not the same as the peak concentration of the tracer mass in the tracer-breakthrough curve, but the more ground-water flow conforms to Fick's law the less obvious the difference between the centroid and the peak concentration.

Mean tracer residence time is estimated from Equation (10) (modified from Gaspar, 1987a, p. 93)

$$\bar{t} = \frac{\int_0^\infty t\, C(t)\, Q(t)\, dt}{\int_0^\infty C(t)\, Q(t)\, dt} \tag{10}$$

with a standard deviation given by Equation (11) (modified from Mull et al., 1988, p. 58)

$$\sigma_t = \left[\frac{\int_0^\infty (t - \bar{t})^2\, C(t)\, Q(t)\, dt}{\int_0^\infty C(t)\, Q(t)\, dt} \right]^{1/2} \tag{11}$$

Equations (10) and (11) assume that tracer residence time will vary from zero for instantaneous exit of the tracer mass from the aquifer system to infinity for tracer mass that is stored in micropores. They provide relevant information on the time required for the centroid of a nonreactive pollutant mass spilled in the vicinity of the injected tracer mass to reach a downgradient receptor.

Mean tracer residence time may be estimated by summation algorithms, a simplified version of which was developed by Mull et al. (1988, p. 56). Their equation provides good results but may be confusing to the uninitiated and may be confused with Equation (10). A simplified example calculation is performed later in this report.

A method for estimating mean tracer residence time was also developed by Smart (1988b) using time-concentration integrals that are based on a routine in Church (1974). This method does not include discharge in the calculation but is generally similar to that presented in this section. This method has not been tested by this author but may be regarded as acceptable.

For contamination studies, initial tracer breakthrough (*i.e.*, first arrival) may be considered more valuable than the tracer residence time, although it may have little theoretical meaning. Initial tracer breakthrough provides ground-water managers with an indication of the length of time a contaminant will take to be detected at a downgradient

receptor. However, because of the effects of longitudinal dispersion, and inadequate sensitivity of current analytical methods at extremely low concentrations renders this situation meaningless.

3.2.2. Mean Tracer Velocity

Mean tracer velocity is a measure of the flow rate of the centroid of the tracer mass and is given by Equation (12) (modified from Gaspar, 1987b, p. 66)

$$\bar{v} = \frac{\int_0^\infty \frac{x_s}{t} C(t)\, Q(t)\, dt}{\int_0^\infty C(t)\, Q(t)\, dt} \tag{12}$$

with a standard deviation given by Equation (13)

$$\sigma_v = \left[\frac{\int_0^\infty x_s \left(\frac{1}{t} - \frac{1}{\bar{t}}\right)^2 C(t)\, Q(t)\, dt}{\int_0^\infty C(t)\, Q(t)\, dt} \right]^{1/2} \tag{13}$$

Tracer migration distance(s) is usually measured as a straight-line distance from the injection point to the tracer recovery sampling station (radial distance = x [L]). A straight-line assumption for karst conduits is unrealistic and should be corrected for sinuosity (Field and Nash, 1997; Worthington, 1991, pp. 85–91) by

$$x_s = 1.5x \tag{14}$$

Estimation of the mean tracer velocity is an appropriate measure of the rate at which the bulk of a nonreactive pollutant mass will migrate in a karst conduit. It also provides a useful insight into the flow hydraulics of the conduit. Equations (12) and (13) also assume that tracer residence time will vary from zero to instantaneous exit of the tracer mass from the aquifer system.

Apparent tracer velocity is a measure of the rate of tracer migration as a function of initial tracer breakthrough; it is obtained by dividing the distance traversed by the tracer cloud by the time of first arrival of the tracer dye. Mean tracer velocity provides substantially improved insight into aquifer functioning over apparent velocity.

Mull et al. (1988, p. 58) provide a simple equation for calculating mean tracer velocity. Their equation is also not reproduced here to avoid confusion. An example of its use is presented later in this report.

3.2.3. Longitudinal Dispersion

Longitudinal dispersion in karst conduits is similar to dispersion in closed conduits and open channels because conduit flow ranges from slow and laminar to rapid and turbulent in karst aquifers that may exhibit either closed-conduit flow or open-channel flow characteristics and similarly for fractured-rock aquifers. The longitudinal dispersion coefficient is a measure of the rate at which a concentrated dye mass spreads out along the flow path (Mull et al., 1988, p. 59). It is defined as the temporal rate of change of the variance of the tracer cloud (Fisher, 1968). It is relevant to the analysis of karst conduits because it provides an indication of the amount of possible spreading of a pollutant mass in terms of increasing persistence and decreasing concentration over time.

Hydrodynamic dispersion, typical of porous media aquifers, may be regarded as not relevant to flow within karst conduits and fractures. Numerous studies on longitudinal dispersion have been conducted over the past few decades (Chatwin, 1971; Sullivan, 1971; Day, 1975; Nordin and Troutman, 1980; Jobson, 1987; Reichert and Wanner, 1991), mostly with respect to open-channel flow. Longitudinal and lateral dispersion for a slug release of tracer or pollutant in a karst conduit (and less so for a fracture) will generally appear as shown in Figure 12. In Figure 12, the responses to a slug of injected tracer are shown *with distance* downstream along selected imaginary streamlines.

As noted by Kilpatrick and Wilson (1989, p. 2), a soluble nonreactive tracer (*e.g.*, some fluorescent dyes) released into a stream behaves in the same manner as the actual water particles. Therefore a measure of the movement of the tracer will in effect be a measure of the movement of an element of fluid in the stream and its dispersion characteristics. It may be further noted that the dispersion and mixing of the tracer in the receiving stream takes place in all three dimensions (Figure 12), although vertical mixing normally occurs before lateral mixing depending on the flow characteristics and velocity variations. Longitudinal dispersion, having no boundaries, continues indefinitely and is the dispersion component of principal interest (Kilpatrick and Wilson, 1989, p. 2).

Longitudinal dispersion is most commonly estimated using the second moment. Dispersion is obtained using Equation (15) (Małoszewski and Zuber, 1992)

$$\frac{D_L}{\bar{v}\, x_s} = \frac{1}{2}\frac{\sigma_t^2}{\bar{t}^2} \tag{15}$$

Equation (15) assumes that Fick's law is always applicable; that is, there is no anomalous behavior. In actuality immobile zones (dead zones) are common, which cause a long tail

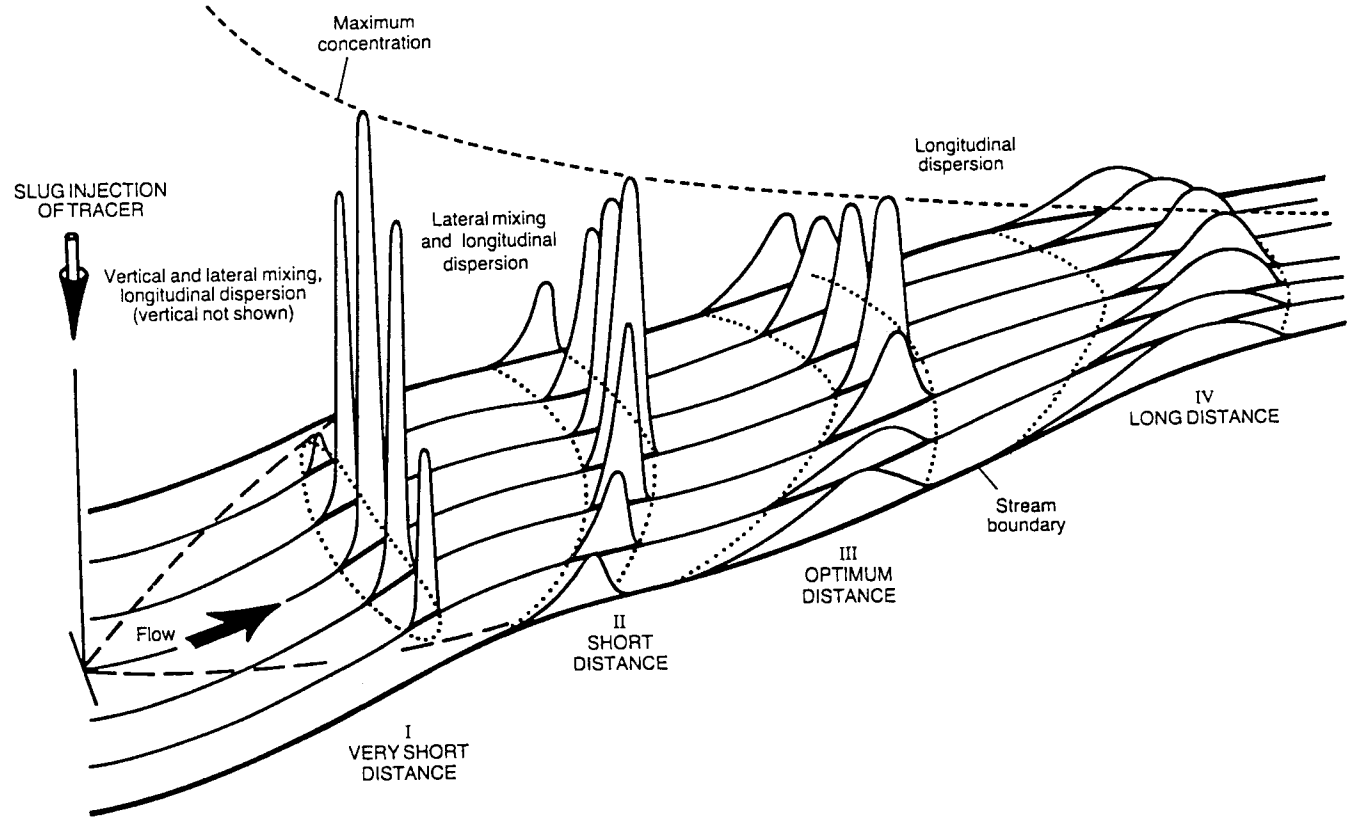

Figure 12. Lateral mixing and longitudinal dispersion patterns and changes in distribution of concentration downstream from a single, center slug injection of tracer (Kilpatrick and Wilson, 1989, p. 2).

to the breakthrough curve and invalidates Fick's law.

Chatwin (1971) developed a method for determining longitudinal dispersion that applies to both closed-conduit flow and open-channel flow. Longitudinal dispersion is given by Equation (16) (Chatwin, 1971) as

$$\left[t \ln\left(\frac{A_p}{C\, t^{1/2}}\right)\right]^{1/2} = \left[\frac{x_s}{2\, D_L^{1/2}} - \frac{\bar{v}\, t}{2\, D_L^{1/2}}\right] \tag{16}$$

The constant of proportionality A_p can be estimated from (Day, 1975)

$$A_p = C_p \sqrt{t_p} \tag{17}$$

The first term on the right-hand side of Equation (16) is the y intercept; the second term on the right-hand side of Equation (16) is the gradient of the line. Either term on the right-hand side allows for solution for the longitudinal dispersion coefficient (D_L) provided that a plot of the left-hand side of Equation (16) against early-time data reasonably falls as a straight line (Day, 1975). The late time data will depart from the straight line due to non-Fickian dispersion characteristics (*e.g.*, dead zones).

Mull et al. (1988, pp. 59–60) developed two equations designed to estimate the longitudinal dispersion coefficient of a karst conduit from dye-tracing studies. Results of the two equations on the same data set produce radically different results. Their Equation 17 appears to be the more reliable estimate for dispersion.

Smart (1988b) developed a relatively simple method of estimating the dispersion coefficient based on the efforts of Brady and Johnson (1981), who used an equation derived by Dobbins (1963). Although not described here, this method appears reasonable and should be considered.

3.2.4. Tracer Dilution

Estimation of tracer dilution in a karst conduit is desirable so that effective dilution of pollutant releases may also be estimated. Given the generally nonconservative behavior of fluorescent tracer dyes and of most pollutants in aquifers as well as their basic differences, estimation of effective dilution is recognized as a very rough approximation at best. Still, estimation efforts can provide useful predictions about potential dilution in the system.

Longitudinal dispersion theory for a conservative tracer, released as a slug at $t = 0$ and $x = 0$ in densely fissured aquifers where dispersion and advection are assumed to be

one-dimensional, suggests that a uniform Gaussian distribution of the tracer concentration will occur in the direction of flow as shown in Equation (9) (Dobbins, 1963)

$$C(x_s, t) = \frac{M_{in}}{A\sqrt{4\pi D_L\, t}} \exp\left[\frac{(x_s - \bar{v}\, t)^2}{4D_L t}\right] \tag{18}$$

Mass M_{in} of the injected tracer is assumed to be small relative to the mass flux rate of the ground water so, in theory, the tracer-breakthrough curve should approach a Gaussian shape. In fact the tracer-recovery curve is always skewed to the right because of the effects of transverse dispersion (ignored in Equation [18]), nonsteady flow conditions, and storage of tracer in very slow-moving water of small voids with later release into large voids, which forms the "tail" of the tracer-breakthrough curve (Atkinson, 1987).

However, tracer behavior is considered to be sufficiently Gaussian-like to allow use of the property of "complementarity." Complementarity suggests that the effects of dispersion on two tracer injections at successive times will proceed independently of each other, and that the combined effect of the two injections will be the sum of their individual effects (Atkinson, 1987). This property was experimentally employed by Smart (1985) to demonstrate the probable dilution estimation for a large quarry that had been used as a landfill for municipal wastes.

Smart derived a dilution equation that utilized tracer input/output concentrations by relating the mass of tracer injected into the aquifer from successive and repeated injections to tracer recovery

$$D = \frac{\bar{C}_i}{C_{pL}} = \frac{M_m}{\Delta t\, Q\, C_{pL}} \tag{19}$$

Steady-state concentration C_{pL} is a function of tracer recovery from a single tracer injection and is given as

$$C_{pL} = \sum_{j=t_b}^{j=t_b+n\,\Delta t} C_j \tag{20}$$

where C_j is the tracer concentration at the resurgence at time j for a single instantaneous tracer injection. Time t_b represents the time between tracer injection and tracer breakthrough at the resurgence. The value, n, equals $d/\Delta t$, where d is the time between tracer breakthrough and final tracer detection at the resurgence (pulse duration).

As may be observed from the above discussion, effective estimation of tracer dilution in a karst aquifer is very difficult. Smart (1985) points out that as the tracer is not conserved in the aquifer, then dilution will be overestimated in proportion to the amount of tracer loss. Effective estimation of tracer dilution is necessary, but much research is still needed.

3.3. KARST CONDUIT AND FRACTURED-ROCK GEOMETRIES

Karst conduit and fracture geometries are estimated by evaluating discharge with respect to mean residence time. This is accomplished for either the continuous or for the discrete situation.

3.3.1. Aquifer Volume

Tracer mass recovery at a spring where discharge was measured during each tracer sampling event allows for a rough estimate of the maximum volume of the conduit or fracture traversed by the tracer cloud by use of Equation (21) (Atkinson et al., 1973)

$$V = \int_0^{\bar{t}} Q\, dt \tag{21}$$

If a single discharge value is used as a mean spring discharge then the karst-conduit volume may be estimated by

$$V = \bar{Q}\,\bar{t} \tag{22}$$

and a total maximum volume estimate based on the sum of each individual conduit or fracture traversed by the tracer cloud may be determined from Equation (23)

$$V_T = \sum_{i=1}^{n} V_i \tag{23}$$

It should be noted that aquifer volume calculations will be only a crude approximation at best. Summing the volumes of individual conduits or fractures to achieve a total maximum volume estimate should not be expected to produce accurate results, but the sum of the individual conduits or fractures does provide some indication of the aquifer volume occupied by conduits or fractures. However, Equations (21) and (22) provide a more realistic estimate of the system volume than could be obtained from the product of mean discharge and time to peak concentration, although this theory requires additional data for confirmation (Smart, 1988b).

By far the majority of volume space will be occupied by micropores, but these contribute little to the flow of ground water in conduit-dominated karst aquifers. As such, it is recommended that investigators consider a variety of methods for estimating aquifer volume and use all the data obtained for a better volume estimation.

Perhaps more valuable is a comparison between inflow rates and outflow rates. If injection discharge is measured during tracer injection, comparisons may be made between

inflow and outflow that may lead to additional insights into the aquifer. For example, inflow/outflow evaluations coupled with comprehensive tracer breakthrough curve analyses furnish a means for assessing the type of karst aquifer under investigation (Atkinson et al., 1973).

3.3.2. Cross-Sectional Area

The easiest and probably most reliable geometric parameter that can be estimated is cross-sectional area. Because the volume V could be estimated from Equations (21) or (22) the cross-sectional area may be estimated from

$$A = \frac{V}{x_s} \tag{24}$$

which is based on a sinuous distance and hence is less than the straight-line distance would suggest.

3.3.3. Karst Conduit Diameter

By assuming a cylindrical karst conduit it is possible to estimate a karst conduit diameter from a tracer-breakthrough curve. Because the system volume has been estimated the karst conduit diameter may be obtained by

$$D_C = 2\sqrt{\frac{A}{\pi}} \tag{25}$$

Obviously $D_C/2$ can be used to estimate the karst conduit radius which is typically used in many modeling endeavors.

3.3.4. Karst Conduit Hydraulic Depth

If open channel flow is assumed to occur in the karst conduit then a hydraulic depth may be estimated by

$$D_H = \frac{A}{D_C} \tag{26}$$

which is a reasonable approximation.

3.3.5. Karst Conduit Surface Area

If the karst conduit is assumed to conform to a cylinder and conforms to Karst Network Types I, II, VI, and VII, then it is possible to obtain an initial estimate of the conduit

surface area. A karst conduit surface area estimate is obtained by

$$A_s = 2\pi r x_s m \tag{27}$$

The roughness correction factor m is necessary because the cylinder concept assumes a "smooth as glass" cylinder. Roughness factor estimation is not straightforward and requires some degree of professional judgment, especially if the karst conduit of interest cannot be directly entered for physical measurements of roughness to be taken.

A reasonable estimate for the roughness factor may be obtained by

$$m = \frac{\varepsilon}{\delta/10^3} \tag{28}$$

The surface irregularities relief ε, taken as 1.0 m, is considered reasonably representative of typical karst conduit walls. There is some support for this assumption from natural river beds (Chow, 1959, p. 196). The laminar flow sublayer δ is divided by 10^3 in Equation (28) to correct for obstructions in the flow regime created by scallops, differential dissolution, large bends, undercut walls, breakdown, and backwater zones as well as other possible flow restrictions. These effects were considered by Atkinson (1977) to explain an estimated roughness height equal to nearly three times the diameter of the karst conduit he was investigating.

3.3.6. Tracer Sorption Estimation

Sorption to karst conduit walls can be estimated by considering a laboratory column as analogous to flow through a karst conduit. Although far from perfect, it can provide useful information for comparison with more theoretically based models.

Karst conduit sorption is estimated by

$$K_a = \frac{(C_0 - C_f)V}{C_f A_s} \tag{29}$$

and for multidischarge karst aquifers (Karst Network Types III and IV)

$$K_a = \frac{(C_0 - C_f)\sum V_i}{C_f \sum A_{s_i}} \tag{30}$$

If a multidischarge karst aquifer is of interest it is essential to note that any results obtained by Equation (29) will be erroneous. Only those results obtained by Equation (30) should be considered relevant.

3.4. EMPIRICAL FLUID DYNAMICS MODELS

Experiments on fluid dynamics have led to the development of many models for flow for specific geometries. These geometries will not necessarily be reproduced by the karst conduits or fracture systems and cannot be reliably approximated whether physical measurements can be taken or not. However, by making some simple assumptions, reasonable parameter estimates may be obtained. For karst conduits, it may be assumed that the phreatic conduit will best be approximated by assuming a cylindrical conduit. Such an assumption is not unreasonable for phreatic conduits developed in flat lying sediments and may not be too unreasonable for other structural and stratigraphic conditions.

3.4.1. Peclet Number

The Peclet number is a measure of the relative contribution of mechanical dispersion and diffusion to solute transport. It relates the effectiveness of mass transport by advection ($-\frac{\bar{v}x_s}{D_{x_s}}\frac{\partial C}{\partial x_s} = -Pe\frac{\partial C}{\partial x_s}$) to the effectiveness of mass transport by either dispersion or diffusion ($\frac{\partial^2 C}{\partial x_s^2}$) (Schiesser and Silebi, 1997, p. 372). Peclet numbers below 0.4 indicate diffusion control; $0.4 - 6.0$ suggests that diffusion and advection are in transition and thus approximately equal to each other; and > 6.0 indicates advection control (Fetter, 1992, pp. 54–55). In most instances of solute transport in karst conduits, Peclet numbers will be greater than 6.0. Often, the Peclet numbers will be many times greater than 6.0.

Estimation of a Peclet number can be obtained from the calculated dispersion and mean tracer velocity from

$$Pe = \frac{\bar{v}\, x_s}{D_{x_s}} \tag{31}$$

It is necessary to note that estimation of the Peclet number by Equation (31) will probably be too low. Substitution of the peak flow velocity v_p could be considered, but most likely would result in overestimating the Peclet number.

3.4.2. Dynamic Flow Equations

Open-channel and closed-conduit flow phenomena are usually described by dimensionless equations for flow behavior. The Reynolds number furnishes a means for determining if flow is laminar or turbulent. The Froude number is used to determine if the flow is subcritical or supercritical.

Reynolds Number The resistance of flow depends entirely upon the geometry and magnitude of the quantity $\frac{\rho \bar{v} d}{\nu}$, where ρ represents fluid density, d conduit diameter, and ν dynamic viscosity. The Reynolds number is the parameter describing the process. The smaller the Reynolds number, the more resistance to flow. Assuming a cylindrical conduit, a rough approximation of the Reynolds number for each individual sampling station may be obtained from

$$N_R = \frac{\rho \bar{v} D_C}{\nu} \tag{32}$$

Estimation of the Reynolds number by Equation (32) will be only a crude approximation because the quantity, $(V/x_s)^{1/2}$, is dependent upon a maximum volume estimate and a straight-line radial distance to the sampling station. Consequently, V is immoderately large, x_s is immoderately small, and $(V/x_s)^{1/2}$ is excessively large. Therefore, calculation of Reynolds number by Equation (14) should be regarded as an upper limit. However, the quantity, V/x_s, has been used to reasonably estimate the cross-sectional area of a single uniform water-filled karst conduit in the Malign karst system (Smart, 1988b).

If the Reynolds number indicates flow to be in the laminar regime, then an equivalent hydraulic conductivity K for flow within the conduit (or conduit) may be calculated. For laminar flow in a karst conduit K is obtained by

$$K = \frac{D_C^2 \rho g}{8\mu} \tag{33}$$

and for laminar flow in a fracture K is obtained by

$$K = \frac{n_e w^2 \rho g}{12\mu} \tag{34}$$

It should be noted that a hydraulic conductivity estimated by either Equation (33) or (34) will be extremely large. In truth K will be approaching infinity (imagine the value of K for a lake). Hydraulic conductivity cannot be approximated for turbulent conditions because, by definition, turbulent flow is a nonlinear phenomenon.

Froude number The ratio of the mean flow velocity to the linear dimension of flow (hydraulic mean depth) is a measure of the extent to which gravitational acceleration affects flow; gravity becomes less important as the ratio increases. Such a ratio is useful for determining if flow is in the subcritical or supercritical range. The parameter describing the effect is the Froude number and is given by

$$N_F = \frac{\bar{v}}{\sqrt{g D_H}} \tag{35}$$

Estimation of the Froude number by Equation (35) will be a rough approximation mainly for the same reasons that apply to the Reynolds number estimation. The Froude number is used to explain flow behavior for streams with a free surface, which may increase uncertainty because karst conduits may exhibit either open-channel flow, closed-conduit flow, or both flow types depending on stage. An estimated Froude number for karst conduits exhibiting closed-conduit flow is not appropriate. Also, as presented the calculation for the Froude number assumes that the cross-sectional area of the karst conduit divided by the diameter of the karst conduit is equal to the mean hydraulic depth, which may not always be true.

3.5. BOUNDARY-LAYER EFFECTS

While not generally considered in tracing studies, boundary-layer effects can substantially impact the study results. In most instances, karst conduit and fracture walls are assumed to be smooth, which is unreasonable. Cave exploration and fractured-rock studies have revealed that conduit walls are often covered with scallops, making them very rough. Additionally, sediment coating on cave walls and layering on cave floors greatly adds to roughness and surface area. Cave breakdown is an extreme case causing significant roughness.

3.5.1. Friction Factor Estimation

When flow is believed to be laminar, a friction factor may be estimated by (White, 1988, p. 163)

$$f_f = \frac{64}{N_R} \tag{36}$$

and for when flow is turbulent, a friction factor may be estimated by (White, 1988, p. 163)

$$\frac{1}{\sqrt{f_f}} = 2\log\frac{D_C}{\varepsilon} + 1.14 \tag{37}$$

where the relief of surface irregularities ε is a controlling factor and depends on the nature of the conduit through which flow is occurring.

3.5.2. Laminar Flow Sublayer

It is well documented by empirical studies that turbulent flow occurs as a core that is surrounded by a laminar flow sublayer. The thickness of the laminar flow sublayer is

dependent on the degree of conduit wall roughness. If a typically very rough karst conduit is assumed, then the laminar flow sublayer may be estimated by (White, 1988, p. 163)

$$\frac{\delta}{D_C} = \frac{32.8}{N_R\sqrt{f_f}} \tag{38}$$

which is an important parameter for assessing the extent of solute sorption to conduit walls and the possibility of matrix diffusion effects. Matrix diffusion can only occur from the laminar flow sublayer.

3.5.3. Hydraulic Head Loss

When flow is laminar, the hydraulic head loss along the conduit can be estimated by (modified from White, 1988, p. 162)

$$h_L = \frac{8.04\mu\bar{v}x_s}{\rho g r^2} \tag{39}$$

and for when flow is turbulent, the hydraulic head loss along the conduit may be estimated by (White, 1988, p. 163)

$$h_L = \frac{f_f x_s \bar{v}^2}{4gr} \tag{40}$$

which emphasizes the influence of friction on head loss.

3.5.4. Shear Velocity

The shear velocity for flow through a karst conduit is created by boundary-layer effects produced by the conduit walls. Therefore it might be expected that the shear velocity will be somewhat less than the flow velocity in the center of the conduit.

Estimation of the shear velocity is obtained by

$$\upsilon_s = \sqrt{g\frac{A}{D_C}\frac{h_L}{x_s}} \tag{41}$$

It will be noted that flow velocities produce by Equation (41) will always be less than those produced by Equation (12). This makes sense in that the karst conduit walls should impart some negative influence on the flow velocity.

4. EXAMPLE CALCULATIONS FOR TOTAL TRACER RECOVERY

To determine the total recovery of tracer injected into an aquifer, the following steps must be initiated. The example calculations describe a scenario in which time is measured in hours and discharge calculations are in SI units to facilitate the explanation. Simple modifications to the procedure may be made for units that vary from the example shown.

1. Plot the Concentration

Subtract background tracer concentration. Plot the concentration of tracer recovered (*e.g.*, mg L^{-1}) verses time in appropriate units (*e.g.*, h). Time should be plotted on the x axis.

2. Plot the Discharge

If the tracer is being recovered at a spring or well where discharge is variable over the time of tracer recovery, then plot discharge in appropriate units (*e.g.*, m^3 s^{-1}) verses time (hours) also. Again, time should be plotted on the x axis. If discharge is constant, then there is no need to plot discharge.

3. Integrate Recovery Curve

Quantitation of tracer recovery is found by integrating everywhere underneath the tracer recovery curve according to Equation (7), which must be integrated numerically. This is done using a simple summation algorithm. This is most easily accomplished by setting up a table which facilitates the necessary calculations (Table 3).

4. Integrate Recovery Curve Again

Integrating the recovery curve a second time, but this time including time t and dividing by the mass recovered (step 3 above) according to Equation (10), will yield the mean residence time. This is most easily accomplished by using the table created in step 3 above, which facilitates the necessary calculations (Table 3).

Table 3. Table representing tracer recovery data for processing.

t (T)	Q (L^3 T^{-1})	C (M L^{-3})	$C \times Q$ (M T^{-1})	$t \times C \times Q$ (M)

Time is recorded in equally spaced increments. If discharge was constant during the

period of tracer recovery, then the Q column of the table has a constant value as well. The $C\,Q$ column is obtained from the product of the second and third column values. The $t\,C\,Q$ column is obtained from the product of the $C\,Q$ column with the t column and by applying appropriate conversions as necessary (*e.g.*, hours vs. seconds).

5. Calculate Tracer Mass Recovery

When the table of values is complete, Equation (7) can be solved by summing column 4 and multiplying by a time conversion to get units of mass only. Hence, the solution to Equation (7) is acquired in a simplified manner by

$$M_O = \int_0^\infty Q(t)C(t)dt \approx \sum_{i=1}^{n} Q_i C_i \Delta t_i \approx t_c \sum_{i=1}^{n} (Q_i C_i) \tag{42}$$

where t_c is any necessary time conversion factor to allow for units of mass.

6. Calculate Mean Tracer Residence Time

Mean tracer residence time $\bar{t}$ is found by solving Equation (10). Equation (10) is solved by the same method that Equation (7) is solved; by simplified summation of the data. From Table 3 sum the values in column five and multiply this value by the appropriate conversion factor to get units of concentration–time. Divide the mass obtained in step 5 above into this number to obtain units of time.

7. Calculate Mean Tracer Velocity

Divide the distance traversed by the tracer cloud by the mean tracer residence time to obtain mean tracer velocity.

8. Repeat for Subsequent Sampling Stations

Repeat the above steps for all wells and/or springs in which the tracer was recovered.

9. Calculate Total Tracer Mass Recovery

If several wells and/or springs recovered the tracer, then sum the individual masses obtained for each well and each spring together to obtain the total tracer mass recovered.

10. Calculate Percent Mass Recovered

Calculate the percentage of mass recovered by dividing the quantity of tracer mass recovered by the quantity of tracer mass injected and multiplying by 100.

4.1. SIMPLIFIED EXAMPLE CALCULATION

Four hundred and thirty-five kilograms of sodium chloride, NaCl, (264 kg Cl^-) (RCA, 1992) were injected into the north coast karst aquifer at the RCA del Caribe (Barceloneta, Puerto Rico) Superfund site for a tracing study. Recovery was at an observation well 120 feet from the injection well that was pumped at a constant rate of 6.0 gpm. Figure 13 displays the tracer-breakthrough curve for the RCA del Caribe Superfund site and Table 4 displays the tracer recovery data and estimation methods for the zeroth and first moments.

4.1.1. Mass Recovery Example

Tracer mass recovery is found by solving Equation (7) or more simply by Equation (42). Equation (42) is solved for tracer mass recovery by multiplying the measured concentration values by the measured discharge values after correcting for consistent units and then summing the results. Column 4 of Table 4 lists the products of columns 2 and 3 and is summed at the end.

The summed results of column 4 of Table 4 must be multiplied by 3600 seconds because time is recorded in hours, but the analyses used seconds.

$$\begin{aligned}\left(4.85 \times 10^2 \text{ mg s}^{-1}\right)\left(3.60 \times 10^3 \text{ s}\right) &= 1.75 \times 10^6 \text{ mg} \\ &= 1.75 \text{ kg}\end{aligned}$$

As shown, 1.75 kg of Cl^- were recovered. Because 264 kg of Cl^- was injected into the aquifer it is evident that only 0.66% of the original tracer mass was recovered. Clearly a serious mass balance problem exists. It may be noted that Equation (42) is not as precise as Equation (7). However, results obtained by Equation (42) will generally be found to be more than adequate in most instances.

4.1.2. Mean Residence Time Example

Tracer residence time is found by solving Equation (10) or its equivalent discrete form. This is accomplished by multiplying column 4 by column 1 in Table 4 and recording the results in column 5. Summing column 5 of Table 4 and multiplying by 3600 seconds will yield results in units of mass–time

$$\left(1.55 \times 10^7 \text{ mg}\right)\left(3.60 \times 10^3 \text{ s}\right) = 5.58 \times 10^{10} \text{mg s}$$

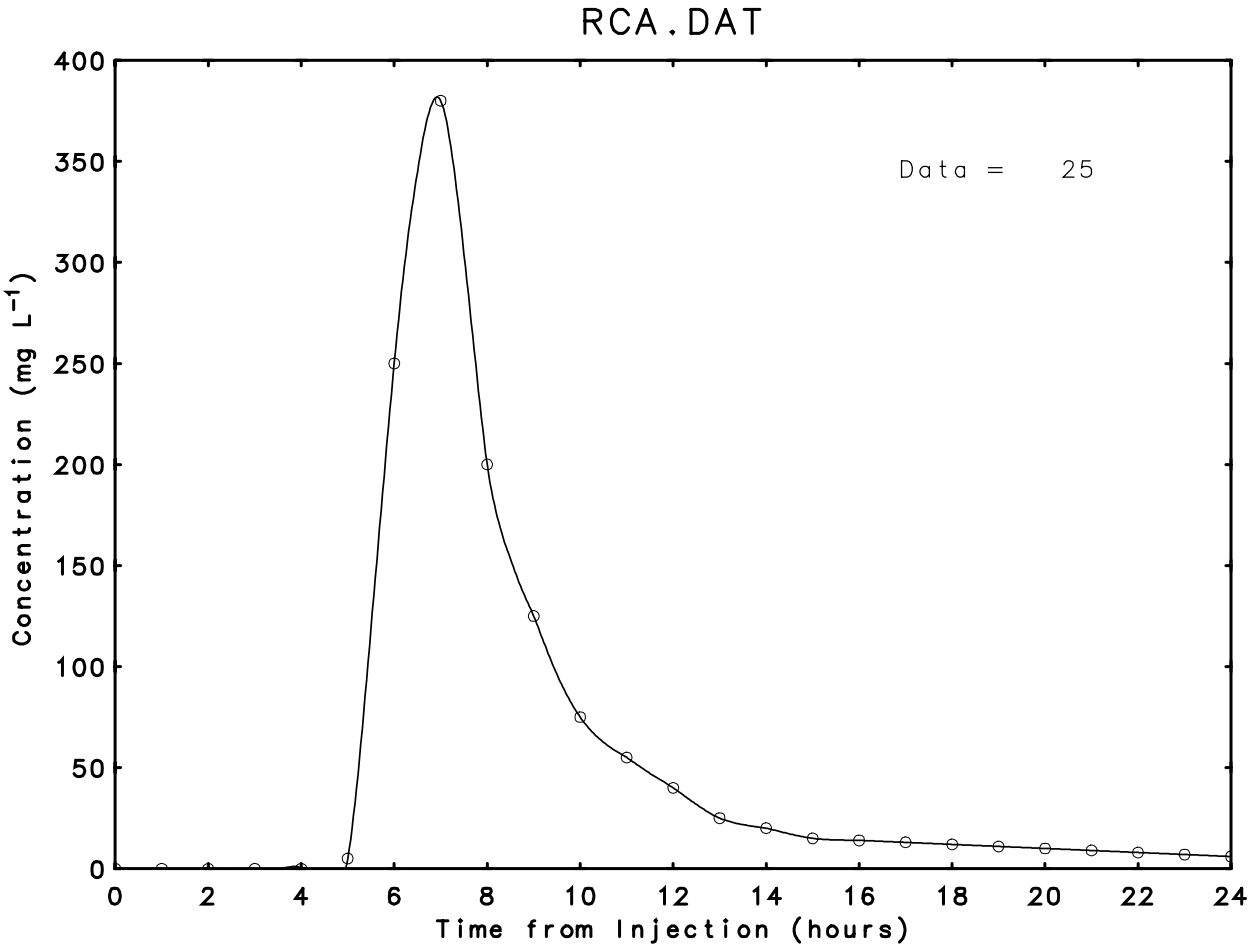

Figure 13. Tracer-breakthrough curve for the RCA de Caribe Superfund site.

Table 4. Spring discharge values and tracer recovery values at specific times.

t (h)	Q ($m^3\ s^{-1}$)	C ($mg\ m^{-3}$)	$C \times Q$ ($mg\ s^{-1}$)	$t \times C \times Q$ (mg)
0.00×10^0	3.79×10^{-4}	0.00×10^0	0.00×10^0	0.00×10^4
1.00×10^0	3.79×10^{-4}	0.00×10^0	0.00×10^0	0.00×10^6
2.00×10^0	3.79×10^{-4}	0.00×10^0	0.00×10^0	0.00×10^6
3.00×10^0	3.79×10^{-4}	0.00×10^0	0.00×10^0	0.00×10^6
4.00×10^0	3.79×10^{-4}	0.00×10^0	0.00×10^0	0.00×10^6
5.00×10^0	3.79×10^{-4}	5.00×10^3	1.90×10^0	3.42×10^6
6.00×10^0	3.79×10^{-4}	2.50×10^5	9.48×10^1	2.05×10^5
7.00×10^0	3.79×10^{-4}	3.80×10^5	1.44×10^2	3.63×10^5
8.00×10^0	3.79×10^{-4}	2.00×10^5	7.58×10^1	2.18×10^5
9.00×10^0	3.79×10^{-4}	1.25×10^5	4.74×10^1	1.54×10^5
10.00×10^0	3.79×10^{-4}	7.50×10^4	2.84×10^1	1.02×10^5
11.00×10^0	3.79×10^{-4}	5.50×10^4	2.09×10^1	8.28×10^5
12.00×10^0	3.79×10^{-4}	4.00×10^4	1.52×10^1	6.57×10^5
13.00×10^0	3.79×10^{-4}	2.50×10^4	9.48×10^0	4.44×10^5
14.00×10^0	3.79×10^{-4}	2.00×10^4	7.58×10^0	3.82×10^5
15.00×10^0	3.79×10^{-4}	1.50×10^4	5.69×10^0	3.07×10^5
16.00×10^0	3.79×10^{-4}	1.40×10^4	5.31×10^0	3.06×10^5
17.00×10^0	3.79×10^{-4}	1.30×10^4	4.93×10^0	3.02×10^5
18.00×10^0	3.79×10^{-4}	1.20×10^4	4.55×10^0	2.95×10^5
19.00×10^0	3.79×10^{-4}	1.10×10^4	4.17×10^0	2.85×10^5
20.00×10^0	3.79×10^{-4}	1.00×10^4	3.79×10^0	2.73×10^5
21.00×10^0	3.79×10^{-4}	9.00×10^3	3.41×10^0	2.58×10^5
22.00×10^0	3.79×10^{-4}	8.00×10^3	3.03×10^0	2.40×10^5
23.00×10^0	3.79×10^{-4}	7.00×10^3	2.65×10^0	2.19×10^5
24.00×10^0	3.79×10^{-4}	6.00×10^3	2.27×10^0	1.96×10^5
		$\sum_{i=1}^{n}$	4.85×10^2	1.55×10^7

(source: RCA, 1992)

and dividing by the mass recovered (1.75 kg) will yield the mean residence time of the tracer in units of time.

$$\begin{aligned} \frac{5.58 \times 10^{10}\ \text{mg s}}{1.75 \times 10^{6}\ \text{mg}} &= 3.19 \times 10^{4}\ \text{s} \\ &= 8.86 \times 10^{0}\ \text{h} \end{aligned}$$

Apparently, it took less than 9 hours for the Cl^- tracer to reach the recovery well.

4.1.3. Mean Tracer Velocity Example

Mean tracer velocity is obtained from Equation (12) or, more simply, by dividing the distance to the sampling station by the time of travel

$$\begin{aligned} \frac{3.66 \times 10^{1}\ \text{m}}{8.86 \times 10^{0}\ \text{h}} &= 4.13 \times 10^{0}\ \text{m h}^{-1} \\ &= 1.15 \times 10^{-3}\ \text{m s}^{-1} \end{aligned}$$

which may then used to estimate the velocity of a nonreactive pollutant, assuming that this value is representative of the prevailing ground-water flow velocity. If the tracer used is of known reactivity with the aquifer, then it may be related to a pollutant of similar reactivity to estimate retardation.

4.1.4. Longitudinal Dispersion Example

Longitudinal dispersion is most accurately estimated by the Chatwin method in Equation (16), which can be tedious.

4.1.5. System Volume

The flow system volume may be estimated using Equation (22). The average discharge for the RCA del Caribe site, 3.79×10^{-4} m^3 s^{-1} (6 gpm), is multiplied by the mean residence time, 3.19×10^4 s, to obtain the system volume.

$$\left(3.79 \times 10^{-4}\ \text{m s}^{-1}\right)\left(3.19 \times 10^{4}\ \text{s}\right) = 1.21 \times 10^{1}\ \text{m}^3$$

Apparently only a small volume of the aquifer was utilized by the tracer to arrive at the recovery well, which was expected given the poor mass recovery.

5. QTRACER COMPUTER PROGRAM DESCRIPTION

To facilitate calculation of total tracer recovery and related information, a FORTRAN computer program has been developed (Field and Nash, 1997). A disk containing the executable file and data files is contained at the end of this document. The program uses a reliable and efficient integration algorithm that takes advantage of an efficient interpolation algorithm (Kahaner et al., 1989, pp. 81–137) and/or extrapolation routines if desired.

5.1. DATA INTERPOLATION

The interpolation algorithm used in the FORTRAN program develops a "piecewise cubic Hermite" function. The interpolant is defined in terms of a set of cubic polynomials, each of which is defined between pairs of consecutive datapoints. The coefficients of these cubic polynomials are chosen so that the interpolant has continuous first derivatives which makes it a "Hermite" interpolant. This is not enough to uniquely determine the interpolant, and the remaining freedom of choice is used to ensure that the interpolant is "visually pleasing," meaning that monotonicity in the data results in monotonicity in the interpolant (*i.e.*, the interpolant does not have extraneous "wiggles"). A piecewise cubic Hermite function in effect produces the most reasonable interpolation of the data possible.

5.2. DATA EXTRAPOLATION

Data extrapolation may be used if tracer sampling ceased prior to complete tracer recovery. Extrapolation may be used to predict the time at which zero (or near zero) tracer concentration would have occurred had tracer sampling been continued until complete tracer recovery was accomplished. The program extrapolates the data by three separate methods.

5.2.1. Exponential Decay

The first and most hydrologically based method uses an exponential decay function in which five additional points are created to produce a reasonably smooth decay curve. This method is based on the concept that most tracer-breakthrough curves in which complete recovery was obtained exhibit exponential decay. Using this method prevents the newly extrapolated data from ever reaching zero (or background) concentration; in reality it would go to infinity if allowed. To overcome this problem the program approximates the best stopping location.

5.2.2. Piecewise Cubic Hermite

The second method relies on the cubic Hermite function to find the single most reasonable stopping datapoint for extrapolation. This is achieved by using the entire tracer-breakthrough curve to develop a smooth function based on the shape of the overall curve and then producing an appropriately chosen extrapolation point. Unfortunately, because the curve has rising and descending limbs and at least one peak (multiple peaks are not uncommon), excessive extrapolation will cause extrapolation to rise incorrectly. A stopping criteria is used to prevent extrapolation from proceeding in a rising fashion, but the net effect is to cause extrapolation to cease prior to zero concentration being reached in most instances. In some instances, even an acceptable decrease may not be achieved.

5.2.3. Straight-Line Projection

The third method for data extrapolation is developed by projecting data for the decreasing limb of the tracer-breakthrough curve beyond the last measured time-concentration data point such that zero tracer concentration is achieved. This is accomplished by projecting a line from the last peak value through each of the measured (or interpolated) data points on the decreasing limb to the x axis and storing the new data point in an array. The greatest cluster of the new data array is then used to estimate a final time value for zero tracer concentration.

5.2.4. Extrapolating Discharge

Extrapolation of discharge data will be a virtual unknown. It is determined here by taking the midpoint of the measured late-time discharge data limb as the endpoint and extending the discharge curve to equal the extrapolated late-time data. If the measured discharge data were decreasing, then the extrapolated discharge data will increase to one-half the original decreasing value. If the measured discharge data were increasing, then the extrapolated discharge data will decrease to one-half the original increasing value.

Extrapolating the data beyond measured values is very risky and may lead to serious errors in the analyses. However, used cautiously, extrapolation of the data may lead to additional insights into aquifer hydraulics.

5.3. CHATWIN'S ESTIMATION OF LONGITUDINAL DISPERSION

Calculation of longitudinal dispersion is accomplished by fitting a straight line through a plot of the Chatwin Parameter versus statistically determined early-time data using an efficient singular value decomposition routine (Kahaner et al., 1989, pp. 218–223), a routine chosen because degenerate data may prevent a straight line calculation by either a least-squares method or by the normal equations. Singular value decomposition always produces a straight-line fit to the data (Vetterling et al., 1992, p. 197). Evaluation of the fit is provided by statistical calculation of the coefficient of determination (R^2), the correlation coefficient (r), the probability of the fit, and Fisher's z statistic. R^2 should approach a value of 1 for a good fit, r should approach a value of -1 for a good fit (for the Chatwin Parameter), the probability of the fit should be a very small value, and Fisher's z statistic may be used in additional statistical tests if desired (Press et al., 1992, pp. 632–633).

Because of memory limitations typical of PCs, there can be instances in which large data files exceed the ability of the data arrays to provide sufficient storage for Chatwin's method of analysis. When this occurs, the method of moments is automatically applied according to Equation (15). Using Equation (15) will almost always result in an overestimation of dispersion, which should be realized.

5.4. DATA NORMALIZATION

Individual tracer tests conducted at the same injection/recovery stations under differing hydrologic conditions should be compared to obtain information regarding aquifer behavior under varying conditions. Normalized tracer concentration files, normalized tracer load files, and standardized tracer concentration files can be calculated by QTRACER and may be analyzed according to the method described by Mull et al. (1988). The discussion by Mull et al. is very comprehensive and as such is not repeated here. Another reason for not repeating the Mull et al. discussion here is because of the probability that in most instances, the ground-water tracing site will (1) have multiple discharge locations, many of which may not be continuously monitored for tracer; and (2) will require more quantitative tracing experiments than can be reasonably undertaken.

5.5. RANGE OF POSSIBILITIES OF QTRACER

QTRACER can be used on almost any type of tracer test in any kind of geological environment (*e.g.*, surface water, porous media, fractured-rock aquifer, or karst aquifer).

This may sound strange, but the statement is true because the basic equations for mass balance are not dependent on geological conditions.

QTRACER was designed to be used in karst systems primarily, but it will handle fractured-rock systems reasonably well when told to do so in the sampling station data file. However, it may be used to evaluate tracer-breakthrough curves from tracer tests conducted in surface water and porous media by entering the relevant information in the sampling station data file(s) and dummy information where the information is irrelevant. The user will then need to note that only some of the output data will make sense.

For example, it would be considered ridiculous to accept the tube diameter output for a tracer test conducted in porous media. However, by exercising some basic judgment, QTRACER can be effectively used in a variety of environments.

5.6. COMPUTER GRAPHICS

A high-quality color graphics algorithm (Kahaner and Anderson, 1990) that includes useful interactive capabilities is included in QTRACER. It provides for visual examination of the data files and other relevant information (*e.g.*, statistics when appropriate). It is particularly useful for evaluating the effect of interpolating and/or extrapolating the original data. Publication quality plots may be generated as postscript files from the graphics screen incorporated into the program. Alternatively, a screen dump using a dot-matrix printer is possible.

5.6.1. Features of the Interactive Graphics Loop

QTRACER takes advantage of a very powerful and useful interactive graphics loop. It is used when a graphics screen is displayed and the user would like to customize the display as desired. The following discussion comes from the user's manual to "Volksgrapher" — *Volksgrapher: A FORTRAN Plotting Package User's Guide, Version 3.0* (Kahaner and Anderson, 1990).

Zooming Type `z` (for "zoom") to enter the zoom mode. Four "zoom corners" will appear for the graph on the screen. The zoom box corners appear on the "current" graph. Use the cursor control keys (arrow keys) to translate the zoom box. To move the zoom box in finer increments, type `f`; to go back to coarse movement, type `c`.

This translates the zoom box; *i.e.*, "whole-moving" mode. Type `s` to enter "side-moving" mode. Typing a cursor control key causes one side of the box to move outward.

To move a side *INWARD*, type a *SHIFTED* cursor control key: *e.g.*, a shifted up arrow moves the top edge down. To get back to "whole-moving" mode, type `w`.

Once the zoom box has been satisfactorily specified, type `z` again to accomplish the zoom. Type `r` to "restore" or "zoom out" to the previous graph (*i.e.*, the one prior to the last zoom). You may zoom in or out several levels.

Press the `Esc` key to remove the zoom box without zooming and return to the normal interactive mode.

Note that zooming will change the mode of all text associated with the graph in mode 2 ("sticking to a point") to mode 1 ("staying a distance from the lower left corner").

Rearranging Graphs Typing `a` (for "arrange") causes four corners to momentarily flash around the "current" graph and places the graphics package into the arrange mode. The space bar, cursor keys, shift keys, and `f`, `c`, `w`, and `s` work as in zoom mode. The current graph will be erased, its new position and shape being indicated only by the corners. To draw the graph in its new position, type `d`. This shifts the graphics package back into "normal" mode.

Typing `x` redraws the entire screen. This is useful when numerous changes have resulted in a cluttered screen. Press `Esc` to leave the arrange mode without changing the graph.

Moving Legends Type `l` (for "legend") to enter the legend moving mode. Corners will briefly flash around the "current" legend. Select legend using the space bar or the backspace key and move the legend around as in the zoom mode. The size of the legend box cannot be changed. Type `d` to draw the currently selected legend, `x` to clean up the screen, or `v` to toggle the current legend between visible and invisible. Press `Esc` to leave the legend mode without changing any legends.

Editing a Graph's Axes Type `e` (for "edit") to change the min/max values on a graph's axes, to switch between linear and logarithmic axes, or to number/unnumber axes. Move the pointer `<` using the cursor keys to select items to change and type `c` to change them. Exit edit mode with `Esc`, which ignores the changes, or type `u` (for "update") to redraw the screen incorporating the changes.

Altering and Adding Text Text strings can be manipulated interactively. New text can be added, even if none of the necessary routines were originally called in the program.

Type `t` to enter text mode; a star will flash at the first letter of the "current" text string. Use the `spacebar` or `backspace` to select a different string. Translate it using the cursor control keys, or rotate it right (clockwise) with `r` or left (counterclockwise) with `l`. The size of the characters can also be changed; they can be made larger by typing "`+`" and smaller by typing "`-`." Type `>` to increase the text's color code and `<` to decrease it. Typing `!` will delete the current text line. To edit the current line, type `e`; you will be prompted for the new contents.

The fineness of translation, rotation and resizing of text can be changed. To go to "fine" movement, type `f`; for "ultrafine," type `u`; to return to "coarse," type `c`.

To change a current string's mode to "keep a distance" mode, type `d`. To change it to "stick to a point" mode, type `p`. To center the current string horizontally, and change its mode to horizontal centering, type `h`. To center the current string vertically, and change its mode to vertical centering, type `v`. To change a string's mode between normal (left) vertical centering and right vertical centering or normal horizontal (bottom) centering and top horizontal centering, type `@`.

To display the current line's color code, number, and positioning mode, type `s` (for "status"). Type `s` again to stop displaying status.

To make the current centered line into an axis label that will act like one entered via the program, type `a`. The current line will then be "owned" by the current graph. The label it becomes depends on its positioning mode: a top-centered line becomes a title, and so forth. If the current line is not centered, it will not become a label.

To add new text, type `n` (for "new"). A prompt will appear, asking for the new line. Entry of the new text line is terminated by pressing the enter key. The new line will have the same size, color, and rotation as the current one and be positioned to line up as the next line "under" it. The new line will have the same positioning mode as the current one, unless the current one is centered. In that case, the new line will have "keep a distance" mode. The new line will be owned by the current graph, *NOT* the current line's owner. The new line becomes the current line, so that blocks of text may be added easily. Note that each page (screen) cannot have more than 50 lines of text. The maximum number of characters in a text string is 70.

To draw a Greek character, precede the letter by `|`. Thus `|a` will draw an α. To subscript or superscript a character, precede it with `_` or `^`. Thus H_2O is the formula for water. Use `^^` to get super-superscript, like e^{x^2} (represents `e` to the `x` squared). To generate a Greek subscript, such as α, use `_|a`. To generate `|`, `_` , or `^` precede it with `|` as in `||sin`

`(x)||`, which will display the absolute value of sin(x) as $|\sin(x)|$.

Some special characters of occasional use (*e.g.*, integral, square root, or arrow) are also available. To access them first look up their THREE-digit ASCII code, then enter the code preceded by a `\`. For example `\202` will produce an integral symbol. To get a backslash, use `\220`.

Type `x` to clean up the screen and return to normal mode. Type `Esc` to leave text mode without redrawing the screen.

Printing The graphics package can produce an output file for PostScript-quality output or dot matrix (Epson-compatible printer). To print a graphics screen to an Epson printer, hit `d`; the screen will be "dumped" to the printer. The default format for high-quality printing is PostScript. This format can be changed in the interactive loop by typing `h`, which then prompts for a device name (those available are listed below):

1. "tek" = Tektronix
2. "hpg" = HPGL-Plotter
3. "pos" = Postscript
4. "qms" = QMS-Lasergrafix

To print the screen, type `p` and provide a *filename*. This file can be sent to an appropriate printer. To send the output directly to a printer on a PC, give the name of the printer port (*e.g.*, `lpt1`) instead of a file name.

Additionally, if the user has requested that the screen display a plot (either data or line or both) and that a PostScript file be generated, a plot file will be created upon exiting the plot screen as occurs when hitting the `ENTER` key.

The Cursor The graphics package has a graphics cursor for finding the position of items on graphs and extracting those values into your program. Type `s` to show the cursor. Then type `w` to display the cursor position in coordinates of the current graph.

Leaving the Interactive Loop Leave the interactive loop by pressing the `ENTER` key. QTRACER will continue after resetting the screen to text mode.

5.7. QTRACER SOURCE

The FORTRAN source for QTRACER is included on the disk. It is a very large program that had to be split into pieces to allow its use on a PC. It is also not recommended that for a user to attempt to follow the logic or to modify the program. Questions regarding the program's functioning can be addressed to the author.

In addition, the graphics routine developed at the National Institute of Standards and Technology includes one C source and one ASSEMBLY source. The ASSEMBLY source is very complicated and not amenable to general manipulation.

6. USING QTRACER

The QTRACER program for tracer-breakthrough curve analysis is an easy-to-use computer package that requires little more of the user than to hit `ENTER` when requested. However, QTRACER requires that data input files be created first for processing. The use of data input files for processing, rather than allowing the user to respond to questions posed by the program, facilitates more rapid data processing while minimizing the opportunities for inputting incorrect data.

6.1. QTRACER PROGRAM AND DATA FILES

Before running the program, you should create a subdirectory on your hard disk for data storage and to protect the original disk. To begin with, please perform the following:

1. At the `C:\>` prompt, type "`MKDIR QTRACER`" (without the quotes — whenever quotes appear in this section type the requested information without the quotes).

2. Next copy the executable and data files from your disk to your hard disk. For example, you might type (if `E` is your disk drive):

   "`COPY E:\*.EXE C:\QTRACER\*.EXE`"
   "`COPY E:\*.DAT C:\QTRACER\*.D`"
   "`COPY E:\*.D C:\QTRACER\*.DAT`"

3. Put your disk in a safe location.

6.2. QTRACER EXECUTION

QTRACER is very easy to use. Once the appropriate data files are created (which are nearly self-explanatory) QTRACER, for the most part, requires nothing more than hitting the `ENTER (RETURN)` key as requested.

1. At the `C:\>` prompt, type "`CD\QTRACER`" without the quotes. You will then see a new prompt; `C:\QTRACER>`.

2. You may now type "`QTRACER`" to run the program by just responding to the requested information and assuming that you have also copied the necessary data files or created your own. You may want to type "`QTRACER` *filename*" such as "`QTRACER ATKIN.D`", which will automatically load and begin running the Atkinson data set described in

the journal article (Field and Nash, 1997). You may do the same with the Mull et al. (1988) data by typing "`QTRACER MULL.D`" which will load the appropriate data files and begin processing.

3. At this point, you will be prompted by the program to enter the file to be evaluated (unless you specified a file when starting the program). One advantage of a subdirectory on your hard disk is that you will not be required to provide an obscure path for all subfiles; the program will find them automatically because they are all at the same location as the executable file. If the data files are in different locations from QTRACER, you will need to provide the correct path to the *.D and *.DAT files.

Additional information will be presented in Section 7. regarding QTRACER execution. However, the really important information (files creation) is listed in this section.

6.3. QTRACER FUNCTIONING

QTRACER runs by processing two types of files at once. The first file called is a header file, which identifies the amount of tracer injected into the aquifer and ALL appropriate subfiles. Subfiles are data files, each of which represents a sampling station where tracer was recovered for the particular study. The subfiles include all necessary information to allow the program to run. They also allow the user to run the program independently of the user (batch mode) or to pause processing to allow the user to observe numerical output and the opportunity to display high-quality graphics. What follows are seven sets of data files that may be used to test the QTRACER Program. If the user so desires, the data files may be reviewed directly, as they are simple ASCII files.

Run QTRACER on each of the supplied files and compare the results with the results provided in the publication "Risk Assessment Methodology for Karst Aquifers: (1) Estimating Karst Conduit-Flow Parameters" (Field and Nash, 1997) [`ATKIN.D` and `MULL.D` only]. Preferably, you will be able to test the program on your own data sets, where you may already know the results. Hopefully your results will compare favorably with those produced by this program.

6.4. SAMPLE FILES ON DISK

The following five "header" data files (*.D) and their respective sample station data files (*.DAT) are included on the disk (Table 5). Each header file must have at least one

corresponding sample station data file that is referenced by the header file. However, the number of sample station data files that correspond to a header file is basically unlimited except as by your computer capabilities.

Note: There is no specific requirement that the data files end with the extensions "D" or "DAT" (*e.g.*, `ATKIN.D`; `ATKIN.DAT`). The "D" and "DAT" extensions are just the convention used in this manual and on the example data file.

Table 5. Example data files on disk.

Header Data File	Sample Station Data File
`ATKIN.D`	`ATKIN.DAT`
`MULL.D`	`MULL.DAT`
`LOST.D`	`LOST.DAT`
`RCA.D`	`RCA.DAT`
`TOPLITA.D`	`TOPLITA.DAT`
`GAR2.D`	`GAR2.DAT`
`MUUL.D`	`MUUL.DAT`

The data files listed in Table 5 are described as follows.

1. `ATKIN.D` and `ATKIN.DAT` are hypothetical data sets provided Dr. Timothy Atkinson (Atkinson, 1987) for educating a group of students (of which this author was one) on the proper methodology for analyzing and interpreting tracer-breakthrough curves. Analysis of these data sets using QTRACER is presented in considerable detail in Field and Nash (1997).

2. `MULL.D` and `MULL.DAT` are data sets taken from a U.S. EPA Region IV report (Mull et al., 1988) in which very comprehensive tracer-breakthrough curve analysis is described. The `MULL.D` and `MULL.DAT` data sets appear slightly modified from the original in that data has been recorded in SI units on the disks. The original Mull et al. data set mixed SI and English units which QTRACER allows for and corrects. Analysis of these data sets using QTRACER is presented in considerable detail in Field and Nash (1997).

3. `LOST.D` and `LOST.DAT` are data sets listing the results of a tracer-breakthrough curve generated by the senior author (and other students) when Dr. Timothy Atkinson was instructing proper methodology for conducting tracer tests and analyzing/interpreting the results. It was obtained for the Lost River Cave System in Kentucky.

4. `RCA.D` and `RCA.DAT` are the data sets that originally inspired the effort to develop QTRACER. A tracer test conducted at an RCA del Caribe Superfund site (Barceloneta, P.R.) supposedly provided substantial information on the functioning of the karst aquifer and on some solute-transport processes in the aquifer. However, only about 0.7% of the Cl^- tracer (injected as NaCl) was recovered. Questions regarding the simple calculations and other factors illustrated in Section 4.1. of this report warranted a more refined approach. This computer program estimates recovery at 0.7%, indicating an extremely poor recovery effort at the site.

5. `TOPLITA.D` and `TOPLITA.DAT` are modified data sets (Gaspar, 1987a, p. 58), the intent of which is to demonstrate that an "ideal" tracer-breakthrough curve is not necessary for QTRACER to function properly. The Toplita data sets are also excellent for demonstrating QTRACER's data extrapolation capabilities because of the shape of the curve and the position of the last measured datapoint.

6. `GAR2.D` and `GAR2.DAT` are modified data sets from a Superfund site in Tennessee. The original data sets were subjected to extensive data interpolation by the computer program NDATA (see Section 9.1. for a description of NDATA). A deliberately "huge" data set was constructed to demonstrate QTRACER's capability of handling data sets that are too large for most PCs. The data set also intended to test the reliability of NDATA's interpolation capability.

7. `MUUL.D` and `MUUL.DAT` are modified data sets of `MULL.D` and `MULL.DAT`, respectively. They were created using NDATA to again assess QTRACER's capabilities of handling "huge" data sets, but with a "variable" discharge (`GAR2.DAT` has a constant discharge).

NOTE: JUST EDIT ONE OF THE *.D FILES AND SAVE AS A NEW FILE WITH A NEW FILE NAME. NEXT EDIT ONE OF THE *.DAT FILES AS OFTEN AS

NECESSARY FOR EACH SAMPLING STATION TO BE ANALYZED AND SAVE EACH AS A NEW FILE WITH AN APPROPRIATELY CHOSEN NEW FILE NAME.

6.5. DESCRIPTION OF *.D FILES

All descriptions in this section use `ATKIN.D` as an example input. An example header file, `ATKIN.D`, appears in Figure 14.

A *.D file (*e.g.*, `ATKIN.D`) is very small. A typical *.D file begins with a requestor for the mass of tracer injected, which should be followed by a value input by the user. Subsequent requestors appear in the same manner as can be seen in Figure 14. That is, a requestor appears, usually with some options that are allowed, so the user will know what can be entered, and the next line is where the user will then enter the appropriate response which will be read by QTRACER. So the first requestor in Figure 14 appears as

```
QUANTITY OF TRACER INJECTED
450
```

which is simply asking for the quantity of tracer material injected into the aquifer. For the `ATKIN.D` example `450` is listed by the user because this was the hypothetical tracer quantity injected into the aquifer.

The file next requests information on the unit of measure for the tracer mass injected, because obviously the number `450` has no meaning without any units.

```
UNITS OF MEASURE (1-lbs, 2-kg, 3-g, 4-mg)
3
```

The numbers enclosed in the parentheses represent the valid units allowed by QTRACER.

```
QUANTITY OF TRACER INJECTED
450
UNITS OF MEASURE (1-lbs, 2-kg, 3-g, 4-mg)
3
SAMPLING DATA FILES LIST
ATKIN.DAT
```

Figure 14. `ATKIN.D` header file for QTRACER processing.

The user should respond with the appropriate units. For the ATKIN.D example a number 3 is listed to indicate grams (g) as the unit of measure.

Lastly, the program asks for the name of all subfiles to be called by QTRACER for processing as part of the *.D file. As previously explained, each header file describing the initial tracer injection conditions must reference at least one sampling station data file, which will be listed here as *.DAT files (*e.g.*, ATKIN.DAT). Thus the subfiles correspond to each sampling station at which tracer was recovered.

```
SAMPLING DATA FILES LIST
ATKIN.DAT
```

For the ATKIN.D example only one station is listed as having recovered tracer, ATKIN.DAT, because that is the only station at which this hypothetical trace recovered the tracer.

If, however, 23 sampling stations had recovered tracer, then all 23 sample files would be recorded here — one above the other, but in no particular order. For example, tracer recovery at 23 sampling stations for the ATKIN.D tracer test might be listed as:

```
 ATKIN.1
 ATKIN.2
 ATKIN.3
    .
    .
    .
ATKIN.23
```

Any other appropriate names such as the names of various monitoring wells or monitored springs are acceptable. The only requirement for the user is that the user be able to recognize the names some time after QTRACER has been run as it will be most advantageous to run QTRACER in the batch mode for large data sets.

6.6. DESCRIPTION OF *.DAT FILES

All descriptions in this section use ATKIN.DAT as example input except as otherwise listed. An example sampling station data file ATKIN.DAT appears in Figure 15.

The *.DAT files (*e.g.*, ATKIN.DAT) are fairly long and detailed. They must be detailed so that the program can properly process all the site information necessary.

6.6.1. Sampling Frequency

A *.DAT file begins by requesting the units used for listing the time data, which must be consistent. The actual time data are listed at the very end of this file along with the concentration data and discharge data when appropriate. So the first item for a *.DAT file

```
SAMPLING FREQUENCY: UNITS (1=days, 2=hrs, 3=min, 4=sec)
2
TRACER RECOVERY CONCENTRATION: UNITS (1=g/L, 2=mg/L, 3=ug/L, 4=ng/L)
3
FLAG FOR BACKGROUND TRACER CONCENTRATION (1/0) AND [VALUE]
0
DISCHARGE IN DATA FILE OR CONSTANT: (1=data file, 2=constant)
1
DISCHARGE: UNITS (1=m^3/d, 2=m^3/hr, 3=m^3/min, 4=m^3/sec, 5=gpd, 6=gpm,
         7=ft^3/d, 8=ft^3/hr, 9=ft^3/min, 10=ft^3/sec) [VALUE]
4
ESTIMATE AQUIFER VOLUME (1=yes, 0=no)
1
RADIAL DISTANCE TO SAMPLING STATION: UNITS (1=m, 2=ft, 3=km, 4=miles) [VALUE]
3 1.8
CORRECTION FOR SINUOSITY (1=yes, 0=no) [VALUE, def=1.5]
1 1.5
CONDUIT OR FRACTURE(S) FLOW,POROSITY (1=conduit, 0=fracture) [VALUE, def=1.0]
1
IF FRACTURE(S) FLOW: UNITS,HEIGHT (1=m, 2=ft, 0=null) [VALUE]
0
NAME OF THE FILE OF INPUT/OUTPUT VALUES
A1.OUT
INTERPOLATE DATA (1=yes, 0=no) [NUMBER OF KNOTS]
0
NAME OF THE INTERPOLATED OUTPUT VALUES FILE
A1.INT
```

Figure 15. ATKIN.DAT sampling station data file for QTRACER processing.

```
EXTRAPOLATE DATA (1=yes, 0=no) [1=EXP. DECAY, 2=CUBIC HERMITE, 3=STAT. METH.]
0 1
VISUALIZATION: STRAIGHT DATA (CHECK PLOT JOIN OPLOT)
0 1 1 0
VISUALIZATION: INTERPOLATED DATA (CHECK PLOT JOIN OPLOT)
0 1 1 0
VISUALIZATION: CHATWIN PARAMETERS (CHECK PLOT OPLOT)
0 1 0
FLAG FOR FILE OF DATA FOR CXTFIT MODELING (CXTFIT Min Mout)
0 0 0
NAME OF FILE FOR SOLUTE-TRANSPORT MODELING (VALID IF FLAG=1)
C:\VANGENU\CXT\A1.ADV
FLAG FOR NORMALIZED CONCENTRATION VALUES FILE (1/0)
1
NAME OF FILE FOR NORMALIZED CONCENTRATION VALUES (VALID IF FLAG=1)
A1.NRM
VISUALIZATION: NORMALIZED CONCENTRATION (CHECK PLOT JOIN OPLOT)
0 0 1 0
FLAG FOR NORMALIZED TRACER LOAD FILE (1/0)
1
NAME OF FILE FOR NORMALIZED TRACER LOAD VALUES (VALID IF FLAG=1)
A1.LOD
VISUALIZATION: NORMALIZED TRACER LOAD (CHECK PLOT JOIN OPLOT)
0 0 1 0
FLAG FOR STANDARDIZED TIME AND CONCENTRATION VALUES FILE (1/0)
1
NAME OF FILE FOR STANDARDIZED TIME AND CONCENTRATION (VALID IF FLAG=1)
A1.STN
VISUALIZATION: STANDARDIZED TIME AND CONCENTRATION (CHECK PLOT JOIN OPLOT)
0 0 1 0
```

Figure 15. `ATKIN.DAT` sampling station data file for QTRACER processing (continued).

```
FLAG FOR OUTPUT TO SCREEN AND PAUSE AS NECESSARY (1/0)
1
FLAG FOR DATA ANALYSIS METHOD (1,ALL DATA; 2,BLOCK AVE; 3,BLOCK SKIP)
3
TIME CONCENTRATION DISCHARGE (CONDITIONAL)
0.0 0.00 4.10
1.0 0.00 4.20
2.0 0.00 4.27
3.0 0.00 4.35
4.0 0.00 4.42
5.0 0.00 4.50
6.0 0.00 4.57
7.0 6.50 4.67
8.0 7.50 4.75
9.0 4.60 4.82
10.0 2.10 4.90
11.0 1.10 4.80
12.0 0.93 4.68
13.0 0.88 4.56
14.0 0.83 4.46
15.0 0.75 4.33
16.0 0.63 4.22
17.0 0.40 4.12
18.0 0.18 4.00
19.0 0.08 3.90
20.0 0.03 3.80
```

Figure 15. `ATKIN.DAT` sampling station data file for QTRACER processing (continued).

is

```
SAMPLING FREQUENCY: UNITS (1=days, 2=hrs, 3=min, 4=sec)
2
```

in which a value of `2` is listed because time was recorded in hours.

NOTE: `SAMPLING FREQUENCY` does *NOT* mean that there must be an even time span between sampling events, only consistent units.

6.6.2. Tracer Mass Recovery

The tracer recovery data must also have consistent units, which follows the same convention as sampling frequency.

```
TRACER RECOVERY CONCENTRATION: UNITS (1=g/L, 2=mg/L, 3=ug/L, 4=ng/L)
3
```

So for the `ATKIN.DAT` example, `3` was recorded because tracer concentration is recorded at the end of this file (corresponding to time data) in units of μg L^{-1}.

6.6.3. Flag for Background

Quite commonly a background concentration value is measured prior to initiating a tracer test. This value must be subtracted from the measured concentration values to allow for a more accurate mass balance estimation.

```
FLAG FOR BACKGROUND TRACER CONCENTRATION (1/0) [VALUE]
0
```

The word "`FLAG`" is a marker that acts like an on/off switch. It informs QTRACER how to respond. The number `0` for the `ATKIN.DAT` data set tells QTRACER that no value for background is available — no "value" is required. The number `1` tells QTRACER that a background value is available for subtracting from the data set — a number `1` *MUST* be followed by a number `[VALUE]` (*i.e.*, concentration) in the *SAME* units as the concentration data set is recorded.

The `[VALUE]` is a requestor that applies only when the `FLAG` is set to `1`, in which case the user *MUST* supply a background concentration for subtraction from the measured concentration values. The user is asked to supply a number **IF** appropriate.

For example, in the `MULL.DAT` example the flag for background appears as

```
FLAG FOR BACKGROUND TRACER CONCENTRATION (1/0) [VALUE]
1 0.01
```

because a background tracer concentration of 0.01 μg L^{-1} is available. This value will automatically be subtracted from all concentration values in the time-concentration data

file prior to processing (but after data interpolation and/or extrapolation). Note that the MULL.DAT data set has already been identified as having tracer recovery concentration values recorded in units equal to μg L^{-1}.

6.6.4. Measured Discharge

Discharge is typically measured as a single occurrence during a tracer test and taken as a constant value, or measured periodically throughout the tracing experiment. QTRACER needs to know which way discharge was measured for proper processing.

```
DISCHARGE IN DATA FILE OR CONSTANT: (1=data file, 2=constant)
1
```

means that for 1=data file, the time-concentration listing at the end of the *.DAT file must also contain a third column of discharge values. The 2=constant means that discharge is a constant whose value must be included in the next section with the discharge units of measure. So for the ATKIN.DAT file a variable discharge 1 is listed, which means that there *MUST* be a third column of data at the end of the ATKIN.DAT data file (Figure 15). If a single (*e.g.*, constant) discharge was recorded then the user would enter 2 on the appropriate line.

6.6.5. Discharge Units

As with all the other data listed, QTRACER needs to know what units discharge was measured in so that an appropriate correction can be made to allow for consistent units. A considerable range of discharge unit measures is allowed by QTRACER, so the requestor actually takes up two lines in the data file.

```
DISCHARGE: UNITS (1=m^3/d, 2=m^3/hr, 3=m^3/min, 4=m^3/sec, 5=gpd, 6=gpm,
        7=ft^3/d, 8=ft^3/hr, 9=ft^3/min, 10=ft^3/sec) [VALUE]
4
```

A number 4 by itself indicates that a variable discharge is recorded in m^3/sec (m^3 s^{-1}), the values of which are listed at the end of the data file (ATKIN.DAT). (QTRACER converts all discharges to m^3 s^{-1}.)

If a constant discharge is to be used (*e.g.*, LOST.DAT) then the user would record

```
DISCHARGE: UNITS (1=m^3/d, 2=m^3/hr, 3=m^3/min, 4=m^3/sec, 5=gpd, 6=gpm,
        7=ft^3/d, 8=ft^3/hr, 9=ft^3/min, 10=ft^3/sec) [VALUE]
4 1.78
```

to indicate that a constant discharge in m^3/sec (m^3 s^{-1}) with a value of 1.78 is to be used in the analysis.

If sampling was performed at a nonpumping well by withdrawing an aliquot of water from the well by use of a bailer, then discharge is unknown (although there is clearly some flux of water flowing past the well). The user should enter a very small flux value unless the flux can be guessed. For example, the user might enter:

```
DISCHARGE: UNITS (1=m^3/d, 2=m^3/hr, 3=m^3/min, 4=m^3/sec, 5=gpd, 6=gpm,
        7=ft^3/d, 8=ft^3/hr, 9=ft^3/min, 10=ft^3/sec) [VALUE]
4 1.0E-10
```

By entering "`4 1.0E-10`" (entering the value `4`, a blank space, and then `1.0E-10`) into the program, the user is multiplying the tracer concentration data file by a very small value so a minimal effect might be applied assuming very little flux past the well (*e.g.*, for tight fissures). Mathematically this works; physically this suggests that discharge is known and is negligible, which may not be correct and may create a fairly substantial error in data analysis.

6.6.6. Aquifer Volume

The aquifer (or flow zone) volume can be estimated by QTRACER provided the time-concentration data file *begins* at zero time. A simple on/off switch informs QTRACER to estimate volume. If the switched is set to off, then subsequent geometries (*e.g.*, cross-sectional area) also will not be estimated.

```
ESTIMATE AQUIFER VOLUME (1=yes, 0=no)
1
```

The switch value `1` for the `ATKIN.DAT` example informs QTRACER that aquifer volume should be estimated.

6.6.7. Radial Distance

QTRACER needs to know the straight-line distance to the sampling station from the injection site and the units by which it was measured.

```
RADIAL DISTANCE TO SAMPLING STATION: UNITS (1=m, 2=ft, 3=km, 4=miles) [VALUE]
3 1.8
```

A distance equal to 1.8 kilometers is entered for the `ATKIN.DAT` example.

6.6.8. Correction for Sinuosity

Because most karst conduits and fractures are not straight-line features, a sinuosity factor may be included for QTRACER to use in processing the data.

```
CORRECTION FOR SINUOSITY (1=yes, 0=no) [VALUE, def=1.5]
1 1.5
```

A listing of `1 1.5` tells QTRACER to correct the radial distance for sinuosity by a factor of `1.5`×. However, because the default is 1.5, a value does *not* need to be entered in this case. The sinuosity factor is limited to a range that is $1.0 < 3.0$.

6.6.9. Conduit or Fracture Flow

QTRACER allows the user to decide if the geometry of the system conforms more to a typical karst conduit (*e.g.*, tubular) or as a fracture (*e.g.*, planar) or set of fractures. If it is a fractured-rock system, then a porosity value will need to be entered by the user as per the `VALUE` request. A default of 1.0 (100%) porosity is used if no value is listed, which suggests that all flow occured via a single fracture. A porosity values has no effect for flow through karst conduits.

```
CONDUIT OR FRACTURE(S) FLOW,POROSITY (1=conduit, 0=fracture) [VALUE, def=1.0]
1
```

For the `ATKIN.DAT` a value of `1` tells QTRACER to consider conduit flow only.

6.6.10. Fracture Geometry Units

If the tracer migrated through a fractured-rock system then the user may want to list the fracture(s) height and the units that the fracture(s) height was recorded. Otherwise, QTRACER will do its best to estimate the height, although the user should not expect the estimated value to be very reliable.

```
IF FRACTURE(S) FLOW: UNITS,HEIGHT (1=m, 2=ft, 0=null) [VALUE]
0
```

The flag `0` is irrelevant here because flow is through a conduit. However, for fracture flow the flag `0` tells QTRACER that fracture height is unknown and must be estimated by QTRACER.

6.6.11. Output File Name

QTRACER requires that an output *filename* be given so that the results may be written to an "out file." The requestor is listed as `INPUT/OUTPUT` because much of the output information is a repeat of input information.

```
NAME OF THE FILE OF INPUT/OUTPUT VALUES
A1.OUT
```

The output file name `A1.OUT` is used here because it allows for easy deletion without

inadvertently deleting the original input files. Any file name is allowed by QTRACER, although the user may not want to use a name that is excessively long, as PCs do not like long file names.

6.6.12. Sample Data Interpolation

QTRACER is very good at data interpolation. It relies on a piecewise cubic Hermit to determine the best possible interpolant for the given data.

```
INTERPOLATE DATA (1=yes, 0=no) and [NUMBER OF KNOTS]
0
```

This requestor is obviously asking if the user would like to interpolate the data. A `0` means NO and the user may move on. A `1` (`ATKIN.DAT` example) means YES and the user then must inform QTRACER of the *MINIMUM* number of knot points to be created by the interpolation algorithm.

If the user would like to have an interpolated data file created the user might record the following.

```
INTERPOLATE DATA (1=yes, 0=no) and [NUMBER OF KNOTS]
1 200
```

The flag and value `1 200`, respectively, inform QTRACER that data interpolation is desired and that ≥ 200 knots points (interpolated data points) are required. Any value other than `200` could be used as your PC memory allows.

6.6.13. Interpolated Data File Name

If an interpolated data file is to be created for processing it must be given a name. This file will be stored and can be viewed later or deleted as desired.

```
NAME OF THE INTERPOLATED OUTPUT VALUES FILE
A1.INT
```

The output file name `A1.INT` is used here because it allows for easy deletion without inadvertently deleting the original input files. Any file name is allowed by QTRACER, although the user may not want to use a name that is excessively long, as PCs do not like long file names. If data interpolation is not requested above, this requestor is ignored by QTRACER.

6.6.14. Sample Data Extrapolation

QTRACER is also very good at data extrapolation, but it is up to the user to determine which method is preferred. That is, the user must decide if an exponential decay function,

a piecewise cubic Hermite, or a straight-line projection from the last peak value through the descending limb is most reasonable. Data extrapolation *requires* that the peak tracer concentration be obtained and that the descending limb of the breakthrough curve be started.

```
EXTRAPOLATE DATA (1=yes, 0=no) [1=EXP. DECAY, 2=CUBIC HERMITE, 3=STAT. METH.]
0 1
```

The `0 1` means that no extrapolation for the `ATKIN.DAT` file is requested (the second flag, `1`, has no effect in this instance).

A `1=EXP. DECAY` means that data extrapolation will be an exponential decay function, a `2=CUBIC HERMITE` means that data extrapolation will be by means of a piecewise cubic Hermite, and a `3=STAT. METH.` means that data extrapolation will be by the statistical method of projecting lines from the peak concentration through the late-time data onto the x axis and determining the greatest cluster.

QTRACER allows the user to extrapolate data to zero or near zero concentration (after subtracting any background tracer concentration) without data interpolation. The user will know the extent of data extrapolation by (1) examining the interpolation data file created if interpolation flag was switched on, or (2) by simply observing the "upper limit" to integration displayed at the top of the final output screen/file. The latter can be observed whether a data interpolation file has been created or not.

6.6.15. Visualize Original Data

The original data may be visually examined before full processing by the user (`CHECK`), plotted as points (`PLOT`), joined by a line (`JOIN`), and directly sent as a postscript plot to a file for later printing (`OPLOT`). Anyone of these four items may be requested or not as desired.

```
VISUALIZATION: STRAIGHT DATA (CHECK PLOT JOIN OPLOT)
0 1 1 0
```

The requestors `CHECK PLOT JOIN OPLOT` are asking if the user would like to:

1. Examine the concentration data file (`CHECK`).
2. Plot the data on the screen (`PLOT`).
3. Draw a smooth line through the datapoints (`JOIN`).
4. Automatically create a postscript output file for plotting (`OPLOT`).

A number `1` answers YES to a requestor, a number `0` answers NO to a requestor. So for the `ATKIN.DAT` example:

```
VISUALIZATION: STRAIGHT DATA (CHECK PLOT JOIN OPLOT)
0 1 1 0
```

tells the program to:

1. Not show the data file (`CHECK = 0`).
2. Plot the data on the screen (`PLOT = 1`).
3. Draw a smooth curve through all the points (`JOIN = 1`).
4. Not create a postscript output file automatically (`OPLOT = 0`).

Data Plotting Each individual plot screen allows for considerable interactive graphics so that the user may customize the plots as desired. The interactive graphics are explained in Section 5.6.1..

Sometimes the curve looks somewhat odd (note odd tip at on the concentration peak for the `MULL.DAT` data set when plotted); this occurs because the Bezier algorithm used for smooth plotting sometimes has difficulty jumping to oddly placed datapoints. Data interpolation by QTRACER will help overcome this effect. Also, fewer than 3 or more than 847 data points will result in no data smoothing.

More importantly, the shape of the curve drawn through the datapoints does not necessarily represent the integration. QTRACER will perform a much better integration of the curve that appears on the screen, in that it will seamlessly connect the points very smoothly even though this function cannot be observed by the user. So the user need not be troubled by the smooth line drawn on screen not appearing to be entirely "perfect."

Automatic Postscript Files Automatic postscript file creation of the plot files is very advantageous when numerous data files must be processed as a batch operation. However, these files will not be produced if the program is set to NOT create a file. This item will usually be set to zero except when QTRACER is being run in batch mode, because the postscript files can be quite large and printing them is unnecessary until a final version based on user modifications is desired.

Be advised automatic postscript output *REQUIRES* that the data *filenames* be NO longer than six characters. A *filename* extension can cause some problems (*e.g.*, *.DAT),

so the automatically created postscript files will be renamed with an underscore (*e.g.*, `ATKIN_01.POS`). The extension *.DAT was not replaced, it just did not fit here because of the name length limitation.

If several postscript files are to be produced (identified in various places in the *.DAT file, QTRACER will number them accordingly. So for the `ATKIN.DAT` example QTRACER might produce six separate postscript files as

`ATKIN_01.POS, . . ., ATKIN_06.POS`

Actually, a long filename with or without an extension can be used, but the designated name of the new data file to be created and listed in the data file must not exceed six characters. In this instance, the program will then create a name `VGnn.pos` where `nn = 01` to `06`.

Manual Postscript Files Postscript files of all screen plots can be created very easily by QTRACER. These will usually be done when QTRACER is not being run in batch mode and after some modifications have been made to the plots to meet a user specified appearance. This is described in considerable detail in a later section.

6.6.16. Visualize Interpolated Data

This requestor is used in the same manner as the previous visualization requestor. The only difference is that it deals with interpolated data only. It functions when data interpolation was requested by the user.

```
VISUALIZATION: INTERPOLATED DATA (CHECK PLOT JOIN OPLOT)
0 1 1 0
```

This example `0 1 1 0` tells QTRACER absolutely nothing for the `ATKIN.DAT` data file because no data interpolation was requested. If data interpolated had been requested, then `0 1 1 0` would tell QTRACER to not display the interpolated data, plot the data with a line on screen, and not produce a postscript plot file.

6.6.17. Visualize Chatwin Parameters

For longitudinal dispersion estimation, QTRACER will first attempt the Chatwin method. If the storage arrays are exceeded, it will go to the method of moments.

The Chatwin parameters are visualized in the same manner as the previous items except for connecting the datapoints with a line. That is, the Chatwin parameters may be examined (`CHECK`), plotted (`PLOT`), and sent to a file as a postscript plot file (`OPLOT`). There

is no JOIN function because the Chatwin method automatically relies on fitting a straight line through the early-time data.

```
VISUALIZATION: CHATWIN PARAMETERS (CHECK PLOT OPLOT)
0 1 0
```

The switches, 0 1 0 for the ATKIN.DAT example, inform QTRACER that the data is to be plotted on the screen only.

6.6.18. CXTFIT2.0 Data File Creation

In some instances, it is possible and desirable to use CXTFIT2.0 (Toride et al., 1995) to model the data. QTRACER facilitates this by allowing the user to automatically create an input file for use with CXTFIT2.0.

Form of CXTFIT2.0 File This option allows the user to request that a CXTFIT file be created (CXTFIT) and that the original injected tracer mass (Min), or the recovered tracer mass (Mout) be used for processing. Determining whether to use the mass injected or the mass recovered is more than just a preference item. It is related to the functioning of the system and the number of recovery stations (*e.g.*, more than one recovery station will usually require Mout), and greatly affects mass balances.

```
FLAG FOR FILE OF DATA FOR CXTFIT MODELING (CXTFIT Min Mout)
0 0 0
```

The three switches 0 0 0 tell QTRACER to not create a CXTFIT2.0 file, and obviously not to use either the mass injected or mass recovered in file creation. If a CXTFIT2.0 file option was set to and the other two options set to zero, then a default of mass injected (Min) would be used.

If a CXTFIT2.0 file is to be created for use in the CXTFIT2.0 model, then the user should:

1. Obtain a copy of the program and the user's manual. CXTFIT2.0 is a very complicated program and requires considerable reading of the manual to understand its functioning.

2. IGNORE all FIRST line data *after* the first item of the CXTFIT2.0 created file — QTRACER adds some additional information for user examination that is not read by CXTFIT2.0.

3. QUESTION initial values for the selected parameters. For example, if QTRACER

was forced to use the method of moments to estimate dispersion, then the "D" parameter listed in the CXTFIT2.0 created file will probably be too large for a global minimum to be found.

These three items are essential before embarking on the use of CXTFIT2.0.

CXTFIT File Name and Location If a CXTFIT2.0 input file is to be created, then the user must give the file a name. Also, if the CXTFIT2.0 program is not stored in the same location as QTRACER, then it is desirable to give it a path to where it should be created so that the user will not need to type in the path to the CXTFIT2.0 file.

```
NAME OF FILE FOR SOLUTE-TRANSPORT MODELING (VALID IF FLAG=1)
C:\VANGENU\CXT\A1.ADV
```

The data line, `C:\VANGENU\CXT\A1.ADV`, tells QTRACER to create the CXTFIT2.0 file at the above listed path where the executable version of CXTFIT2.0 is stored. Actually, this requestor is ignored in this instance because QTRACER was informed above to not create a CXTFIT2.0 file.

It should be noted that any of the files to be created by QTRACER (except as by `OPLOT`) can be given a path for file storage.

6.6.19. Normalized Tracer Mass

The tracer concentration data may be normalized for mass according to the Mull et al. (1988) method. That is, the concentration data may be rewritten into consistent units (mg L^{-1}) kg^{-1} injected to allow for comparison of multiple tracer-breakthrough curves conducted at the same tracer injection-recovery location. This newly created data may also be examined.

Flag to Create Normalized Data File for Mass The creation of a normalized concentration data file is performed by the on/off switch described earlier. A switch of `1`=on and a switch of `2`=off.

```
FLAG FOR NORMALIZED CONCENTRATION VALUES FILE (1/0)
1
```

Name of Normalized Concentration File for Mass As with all other files created by QTRACER, a file name must be provided before QTRACER can create the file.

```
NAME OF FILE FOR NORMALIZED CONCENTRATION VALUES (VALID IF FLAG=1)
A1.NRM
```

A file name with an extension (*.NRM) is not required. Any name is acceptable. The "VALID IF FLAG=1" requestor refers to the above on/off switch.

Visualize Normalized Concentration The newly created normalized concentration file can be visualized in the same manner as the original data. That is, the data can be examined (CHECK), plotted (PLOT), joined with a line (JOIN), and automatically sent to a file in postscript form for postscript plotting (OPLOT).

```
VISUALIZATION: NORMALIZED CONCENTRATION (CHECK PLOT JOIN OPLOT)
0 0 1 0
```

Setting the four switches to 0 0 1 0 tells QTRACER to just display a smooth line on the screen.

6.6.20. Normalized Tracer Load

The tracer concentration data may be normalized for loading according to the Mull et al. (1988) method. That is, the concentration data may be rewritten into consistent units of (mg s^{-1}) kg^{-1} injected to allow for comparison of multiple tracer-breakthrough curves conducted at the same tracer injection-recovery location. This newly created data may also be examined.

Flag to Create Normalized Data File for Loading The creation of a normalized concentration data file is again performed by the on/off switch described earlier. A switch of 1=on and a switch of 2=off.

```
FLAG FOR NORMALIZED TRACER LOAD FILE (1/0)
1
```

Name of Normalized Concentration File for Load As with all other files created by QTRACER, a file name must be provided before QTRACER can create the file.

```
NAME OF FILE FOR NORMALIZED TRACER LOAD VALUES (VALID IF FLAG=1)
A1.LOD
```

A file name with an extension (*.LOD) is not required. Any name is acceptable.

Visualize Normalized Tracer Load The newly created normalized load file can be visualized in the same manner as the original data. That is the data can be examined (CHECK), plotted (PLOT), joined with a line (JOIN), and automatically sent to a file in postscript form for postscript plotting (OPLOT).

```
VISUALIZATION: NORMALIZED TRACER LOAD (CHECK PLOT JOIN OPLOT)
0 0 1 0
```

Setting the four switches to `0 0 1 0` tells QTRACER to just display a smooth line on the screen.

6.6.21. Standardized Data File

The tracer concentration data may be standardized for dimensionless time and concentration according to the Mull et al. (1988) method. That is, time may be rewritten by

$$\frac{(t - \bar{t})}{\sigma_t} \tag{43}$$

and concentration data may be rewritten by

$$\frac{C}{C_p} \tag{44}$$

to create a completely dimensionless tracer-recovery curve that may be used as a "type curve" for future contaminant release problems (see Mull et al. [1988] for a comprehensive discussion). This newly created data may also be examined.

Flag to Create Standardized Data File The creation of a standardized dimensionless data file is again performed by the on/off switch described earlier. A switch of `1`=on and a switch of `2`=off.

```
FLAG FOR STANDARDIZED TIME AND CONCENTRATION VALUES FILE (1/0)
1
```

Name of Standardized Data File As with all other files created by QTRACER, a file name must be provided before QTRACER can create the file.

```
NAME OF FILE FOR STANDARDIZED TIME AND CONCENTRATION (VALID IF FLAG=1)
A1.STN
```

A file name with an extension (*.STN) is not required. Any name is acceptable.

Visualize Standardized Data File The newly created standardized time-concentration file can be visualized in the same manner as the original data. That is, the data can be examined (`CHECK`), plotted (`PLOT`), joined with a line (`JOIN`), and automatically sent to a file in postscript form for postscript plotting (`OPLOT`).

```
VISUALIZATION: STANDARDIZED TIME AND CONCENTRATION (CHECK PLOT JOIN OPLOT)
0 0 1 0
```

Setting the four switches to `0 0 1 0` tells QTRACER to just display a smooth line on the screen.

6.6.22. Screen Display

QTRACER allows for processing interruption for displaying results by use of the on/off switch (`1=on, 0=off`). If the user would like to view the program results as they become available, then the switch should be set to `1`=on. QTRACER will pause periodically to allow the user to view the results; RETURN will inform QTRACER to continue.

Setting the switch to `0`=off allows QTRACER to run in the batch mode. This preferable when many sample station data files must be processed for a single header file.

```
FLAG FOR OUTPUT TO SCREEN AND PAUSE AS NECESSARY (1/0)
1
```

6.6.23. Method for Handling Large Time-Concentration Data Files

With the advent of automatic data loggers, incredibly large time-concentration data files are being recorded. Often these files are much too large for conventional PC memory allocation. Because of this problem, QTRACER has been programmed to adjust accordingly by:

1. Using all the time-concentration data, provided PC memory is not exceeded.
2. Averaging blocks of data to create a single datapoint for each block.
3. Skipping blocks of data.

Obviously the more measured data that QTRACER can handle the better. Therefore, if QTRACER must use less than all the data it will attempt to minimize the size of the blocks it must either average or skip.

```
FLAG FOR DATA ANALYSIS METHOD (1,ALL DATA; 2,BLOCK AVE; 3,BLOCK SKIP)
1
```

Two sets of data files that were created to be "huge" are included on the disk. The first `GAR2.D` and `GAR2.DAT`, were created by interpolation data collected at a Superfund site with constant discharge. The second set, `MUUL.D` and `MUUL.DAT`, were created from the MULL data set by interpolation and include a "variable" discharge (actually, discharge did not vary all the while that it was measured).

6.6.24. Actual Time-Concentration Data

The last item to be listed for each *.DAT file is the actual time-concentration data and discharge data if these were not constant. The actual time-concentration data set (and discharge data if relevant) are recorded in the UNITS identified at the top of the *.DAT file. Discharge is only required to be listed if a variable discharge was measured at each sampling interval. For the `ATKIN.DAT` example:

```
TIME CONCENTRATION DISCHARGE (CONDITIONAL)
0.0 0.00 4.10
      ⋮
20.0 0.03 3.80
```

is listed to correspond with `TIME CONCENTRATION DISCHARGE` measurements. The parenthetical `CONDITIONAL` relates to whether discharge was variable or constant. If discharge was identified as a variable earlier, then a discharge column must be recorded; if discharge was identified as a constant earlier, then a discharge column must not appear.

If a single or average (constant) discharge was measured for the site, a constant discharge value should have been identified earlier in the data file where appropriate. So for the `RCA.DAT` example, only the `TIME CONCENTRATION` values are recorded as:

```
TIME CONCENTRATION DISCHARGE (CONDITIONAL)
0.0 0.0
  ⋮
24.0 6.0
```

Earlier in the `RCA.DAT` data file (near the top), discharge had been identified as being a CONSTANT (flag = `2`) with `UNITS` and `VALUE` equal:

```
6 6
```

which indicates that discharge was recorded in "gpm" (flag = `6`) and the actual discharge value = `6` (second number 6 listed).

Please be advised that the `TIME CONCENTRATION` files do not need to list all the occurrences of zero tracer recovery at the beginning of the tracer study. However, the time `0.0` should be listed at the very top of the data file to indicate the time of tracer injection. If aquifer volumes are to be estimated for a variable discharge `TIME` must begin with `0.0`.

Conduit volume and Reynolds number can only be calculated if discharge was measured at a *SPRING*, not a well. If a well is analyzed and the appropriate flags turned on to indicate

a desire to calculate conduit volume and Reynolds number, both will be calculated, but significant uncertainties should be expected in the results. So for the `RCA.DAT` data sets, these calculations are suspect.

7. EXAMPLE ANALYSES FROM QTRACER

QTRACER is very easy and fast to use once the necessary header file and sampling station data files have been created (see Section 6.). As described in Section 6.2., the user need only type `QTRACER` and hit `ENTER` to initiate QTRACER, which will introduce the program and then ask for the name of a header file (tracing project file). Alternatively, the user could type `QTRACER` *filename*, which will introduce the program and automatically load and begin running the specified header file and subsequent data files.

At this point, QTRACER will proceed along until finished if the batch mode has been specified (see Section 6.6.22.). Alternatively, if the screen display has been requested, QTRACER will pause periodically to allow the user to observe the analytical results as they become available. Simply hitting `ENTER` as directed by QTRACER will cause QTRACER to move on to the next available display screen.

Lastly, if multiple sampling station data files are to be processed by QTRACER for a single tracing project file or header file (see Section 6.5.), then QTRACER will enter a loop mode. Upon completion of processing a single sampling station data file, QTRACER will clear most of its memory and loop back to read and process the next sequentially listed sampling station data file in the header file list. Upon processing all the sampling station data files, QTRACER will then develop a final total output of some specific information (*e.g.*, total mass recovery) and append this small output subfile to the *LAST* specified sampling station output file.

7.1. ATKIN.D EXAMPLE OUTPUT

In Section 6.5. ATKIN.D was used as an example tracing project file or header file. ATKIN.D referenced the sampling station data file, ATKIN.DAT (Section 6.6., and Table 5) that provided all the information necessary for QTRACER processing of the data obtained for that sampling station.

7.1.1. ATKIN.DAT Tracer-Breakthrough Curve

Figure 16 depicts the basic tracer-breakthrough curve generated by QTRACER and analyzed by QTRACER. Note that discharge was measured each time a water sample was collected.

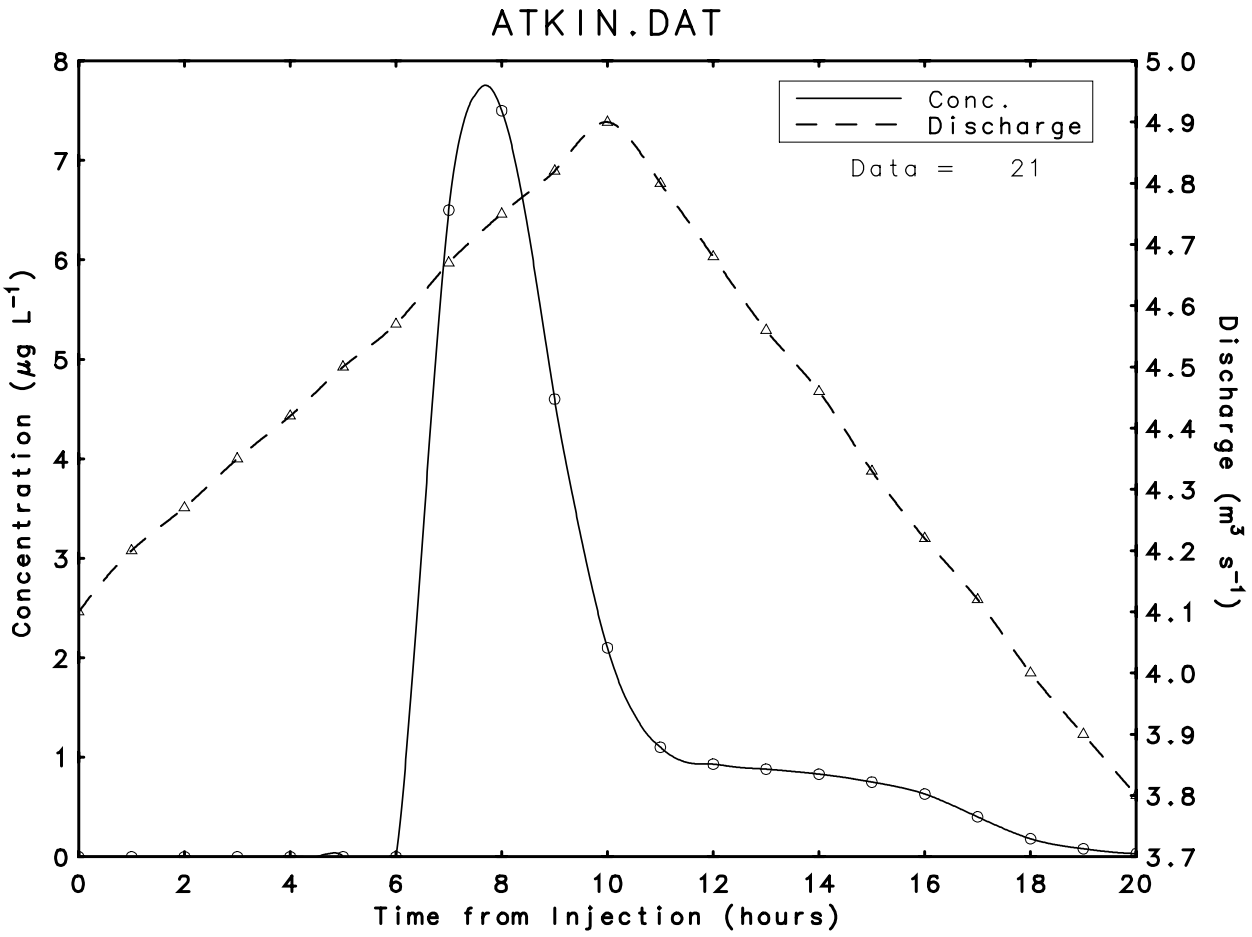

Figure 16. Tracer-breakthrough curve for the ATKIN.DAT sampling station data file.

7.1.2. ATKIN.DAT Chatwin Plot

Figure 17 depicts the data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

7.1.3. ATKIN.DAT Output File

Figure 18 depicts the final analytical output generated by QTRACER. Besides observing the analytical results, note the end of the output file, which depicts the "total" results of the analysis. QTRACER performs this function even though only a single sampling station data file was analyzed. As such, the total results are the same as those listed in the main part of the output file.

7.1.4. ATKIN.DAT Normalized Tracer Concentration

Figure 19 depicts the normalized tracer concentration data generated by QTRACER according to the method described by Mull et al. (1988). Note the concentration units for the y axis.

7.1.5. ATKIN.DAT Normalized Tracer Load

Figure 20 depicts the normalized tracer load data generated by QTRACER according to the method described by Mull et al. (1988). Note the concentration units for the y axis.

7.1.6. ATKIN.DAT Standardized Time-Concentration Data

Figure 21 depicts the standardized-time concentration data generated by QTRACER according to the method described by Mull et al. (1988). Note the time units on the x axis and the concentration units on the y axis.

7.2. RCA.D EXAMPLE OUTPUT

In Section 4.1. a tracer test conducted at the RCA del Caribe Superfund site (Barceloneta, P.R.) was used as an example for analysis. RCA.D is the header file read by QTRACER and references the sampling station data file, RCA.DAT (Table 5), that provides all the relevant information necessary for QTRACER processing of the data obtained for that sampling station.

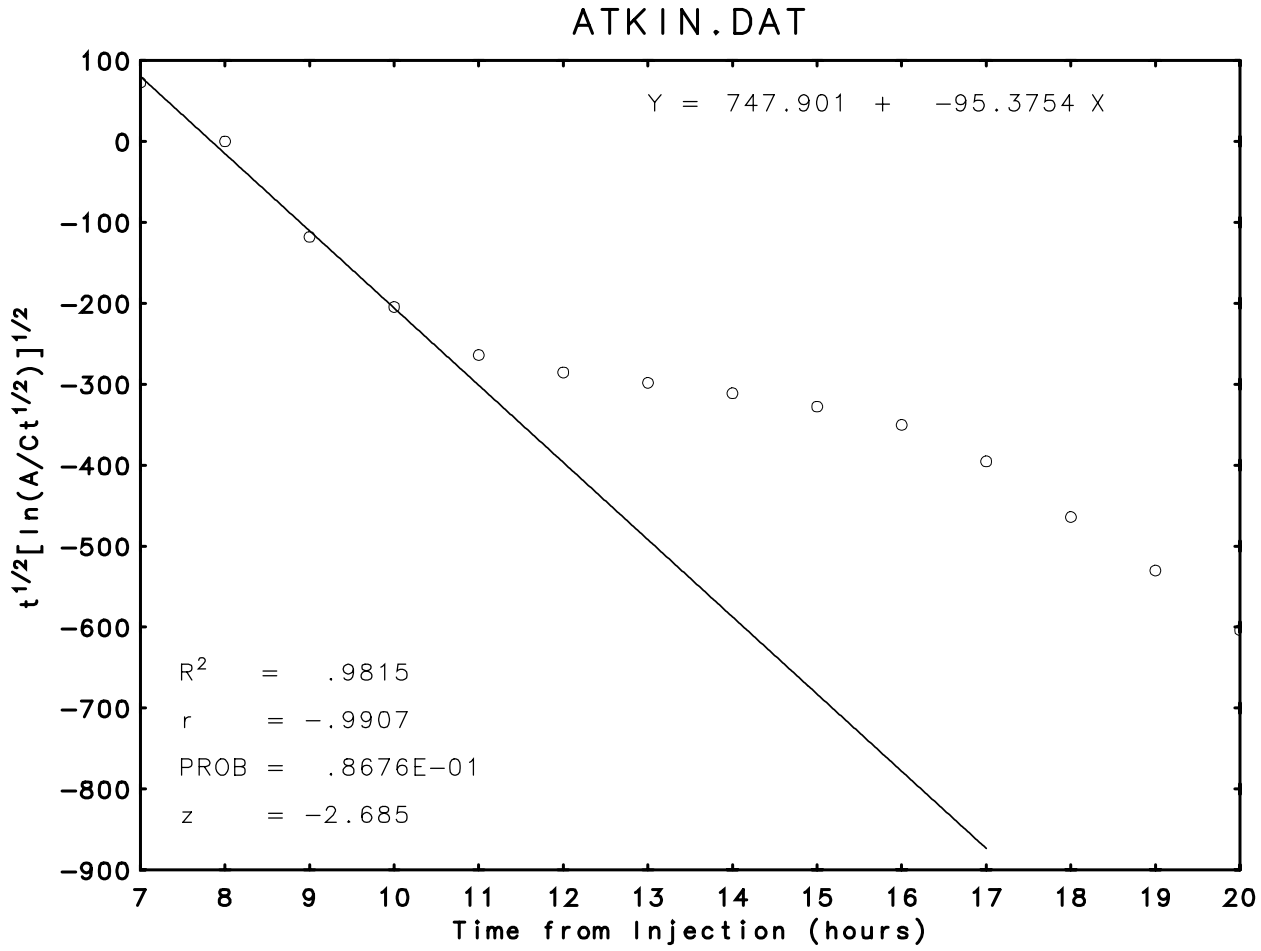

Figure 17. Plot and straight-line fit of the Chatwin parameter for the ATKIN.DAT sampling station data file.

```
**********************************************************************
**********************************************************************

           ------------------------------------

            Listing of output for:  ATKIN.DAT

           ------------------------------------

Limits to integration for the data file:ATKIN.DAT

 Lower integration limit                          .00000      hrs
 Upper integration limit                          20.000      hrs


The quantity of tracer recovered                  .44798      kg
                                                  447.98      g
                                                  .44798E+06  mg
                                                  .44798E+09  ug

Distance from input to outflow point              2.7000      km
Corrected for sinuosity = 1.50X


Time to leading edge (first arrival)              7.0000      hrs


Time to peak tracer concentration                 8.0000      hrs
For a peak tracer concentration                   7.5000      ug/L
```

Figure 18. Output file for the ATKIN.DAT sampling station data file.

```
The mean tracer transit time                    .38629       d
                                                9.271070     hrs
                                                556.2642000  min

Standard deviation for tracer time              .10731       d
                                                2.5754       hrs
                                                154.5220000  min


The mean tracer velocity                        6989.484000  m/d
                                                291.2285     m/hr
                                                .80897E-01   m/s

Standard deviation for tracer velocity          134.51       m/d
                                                5.6047       m/hr
                                                .15569E-02   m/s



Dispersion coefficient                          3.2582       m^2/s
Longitudinal dispersivity                       40.276       m


Peclet number                                   77.688
                                                Advection > Diffusion


The maximum tracer velocity                     9257.143000  m/d
                                                385.7143     m/hr
                                                .10714       m/s
```

Figure 18. Output file for the ATKIN.DAT sampling station data file (continued).

```
Karst-conduit volume estimate                    .14941E+06  m^3
 Based on a lower integration limit              .00000      hrs
 and on an upper integration limit               9.2711      hrs

Karst-conduit cross-sectional area               55.338      m^2
Karst-conduit surface area                       51552650.   m^2
 Tracer sorption coefficient (conduit)           .13046E-04  m

Hydraulic head loss along conduit                .12021E-01  m
 Based on a friction factor                      .11201


Laminar flow sublayer along walls                1.3811      mm
Estimated Reynolds number                        595636.9000
 Based on an estimated tube diameter             8.3939      m


Estimated Froude number                          .10061E-01
 Based on an estimated hydraulic depth           6.5926      m


Shear velocity                                   .16966E-01  m/s


Molecular mass transport parameters
 Estimated Schmidt number                        1140.026000
 Estimated Sherwood number                       14925.68000
 Mass transfer coef. from wall to flow           .17782E-05  m/s
 Molecular diffusion layer thickness             .56238      mm


Percent recovery of tracer injected              99.55       %
Accuracy index (0.0 = Perfect Recov.)            .4481E-02
```

Figure 18. Output file for the ATKIN.DAT sampling station data file (continued).

```
**********************************************************************
**********************************************************************

     ------------------------------------------

       Listing of total estimates for:  atkin.d

     ------------------------------------------

Total quantity of tracer recovered                  .44798      kg
                                                    447.98      g



Total aquifer volume estimate                       .14941E+06  m^3

Total aquifer surface area estimate                 51552650.   m

Final tracer sorption coefficient                   .13046E-04  m


Percent recovery of tracer injected                 99.55       %
Accuracy index (0.0 = Perfect Recov.)               .4481E-02
```

Figure 18. Output file for the `ATKIN.DAT` sampling station data file (continued).

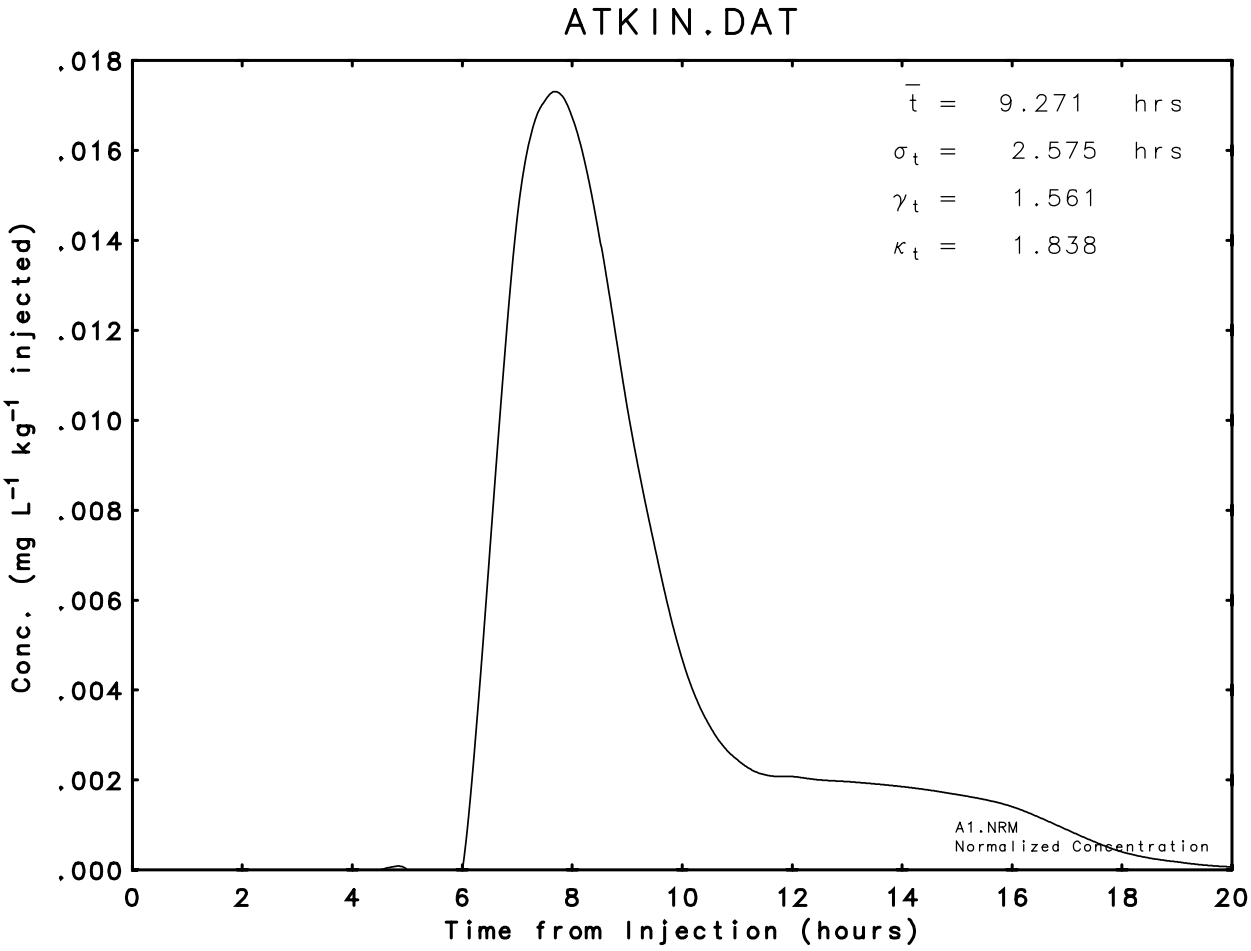

Figure 19. Normalized tracer concentration data for the ATKIN.DAT sampling station data file.

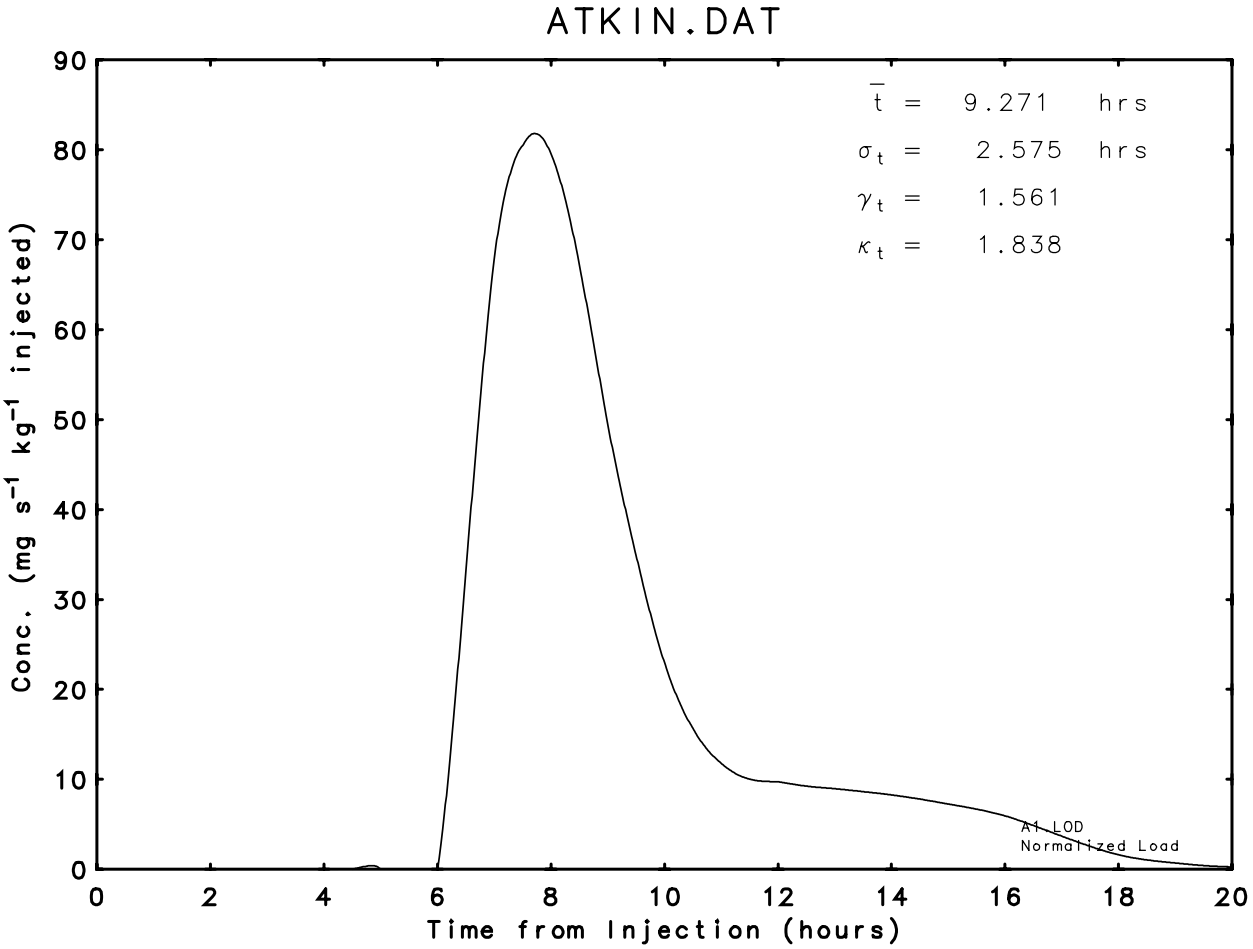

Figure 20. Normalized tracer load data for the ATKIN.DAT sampling station data file.

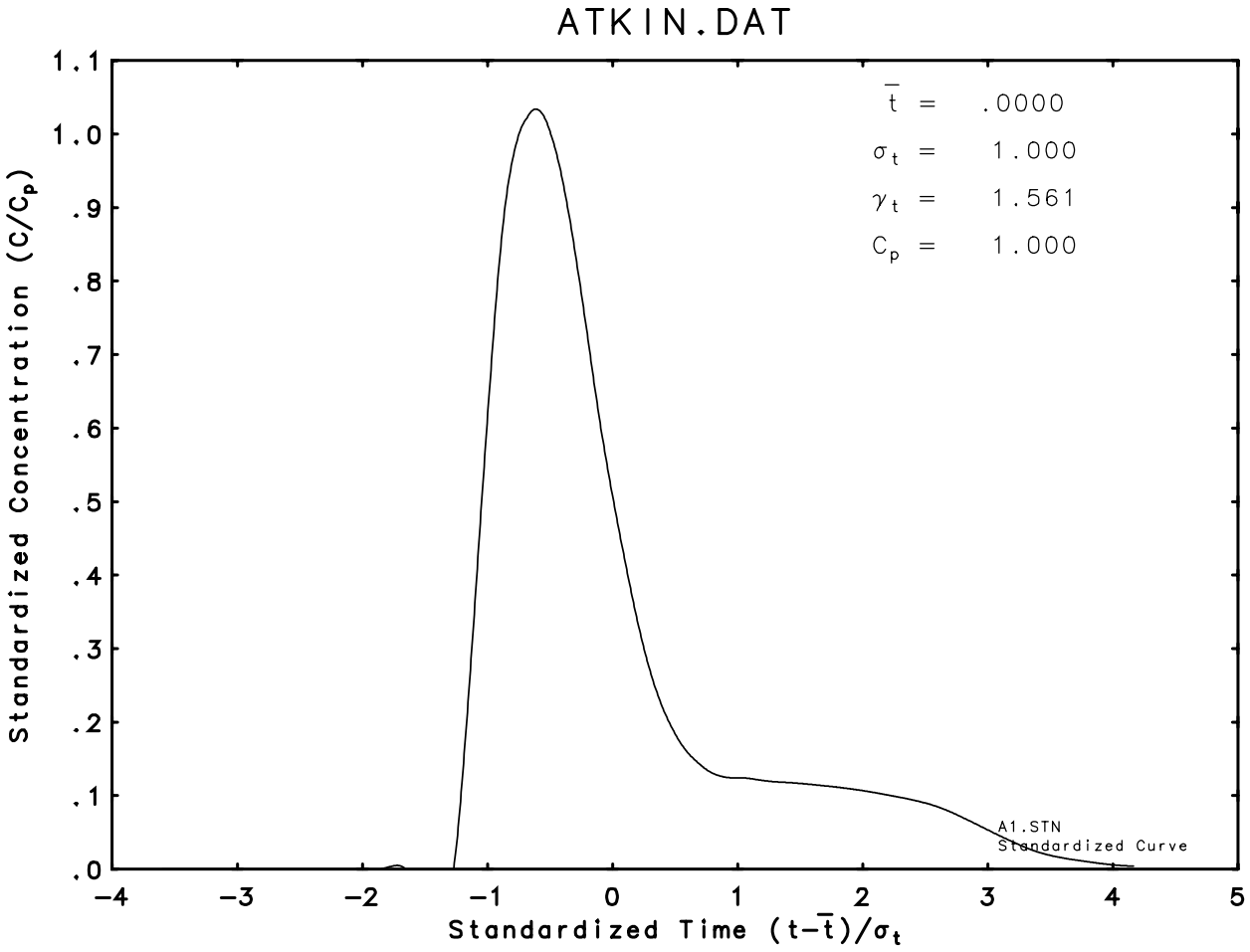

Figure 21. Standardized time-concentration data for the ATKIN.DAT sampling station data file.

7.2.1. RCA.DAT Tracer-Breakthrough Curve

Figure 22 depicts the basic tracer-breakthrough curve generated by QTRACER and analyzed by QTRACER. Note that discharge was measured each time a water sample was collected.

7.2.2. RCA.DAT Chatwin Plot

Figure 23 depicts the data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated by QTRACER and analyzed by QTRACER. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

7.2.3. RCA.DAT Output File

Figure 24 depicts the final analytical output generated by QTRACER. Besides observing the analytical results, note the end of the output file, which depicts the "total" results of the analysis. QTRACER performs this function even though only a single sampling station data file was analyzed. As such, the total results are the same as those listed in the main part of the output file.

7.2.4. RCA.DAT Normalized Tracer Concentration

Figure 25 depicts the normalized tracer concentration data generated by QTRACER according to the method described by Mull et al. (1988). Note the concentration units for the y axis.

7.2.5. RCA.DAT Normalized Tracer Load

Figure 26 depicts the normalized tracer load data generated by QTRACER according to the method described by Mull et al. (1988). Note the concentration units for the y axis.

7.2.6. RCA.DAT Standardized Time-Concentration Data

Figure 27 depicts the standardized-time concentration data generated by QTRACER according to the method described by Mull et al. (1988). Note the time units on the x axis and the concentration units on the y axis.

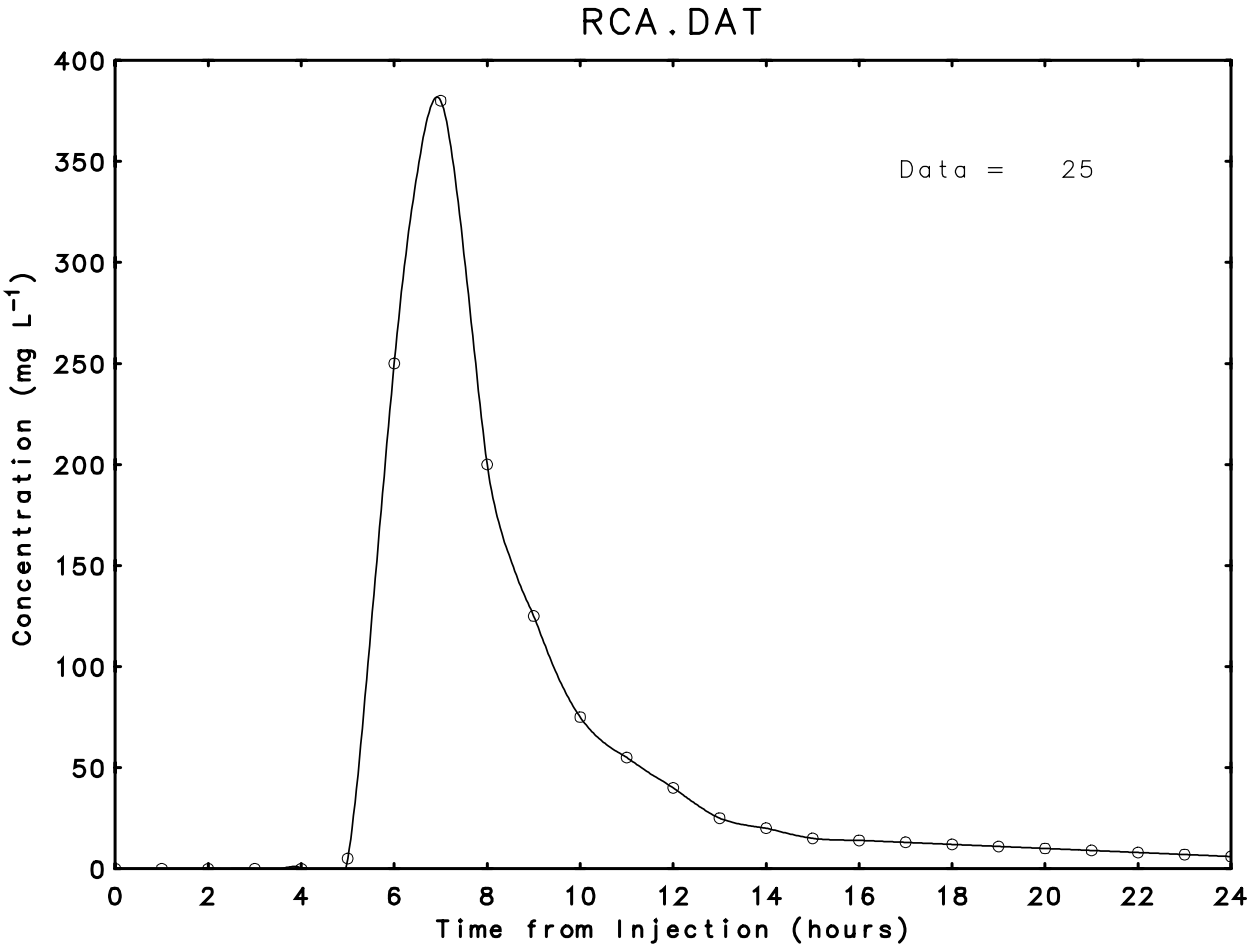

Figure 22. Tracer-breakthrough curve for the RCA.DAT sampling station data file.

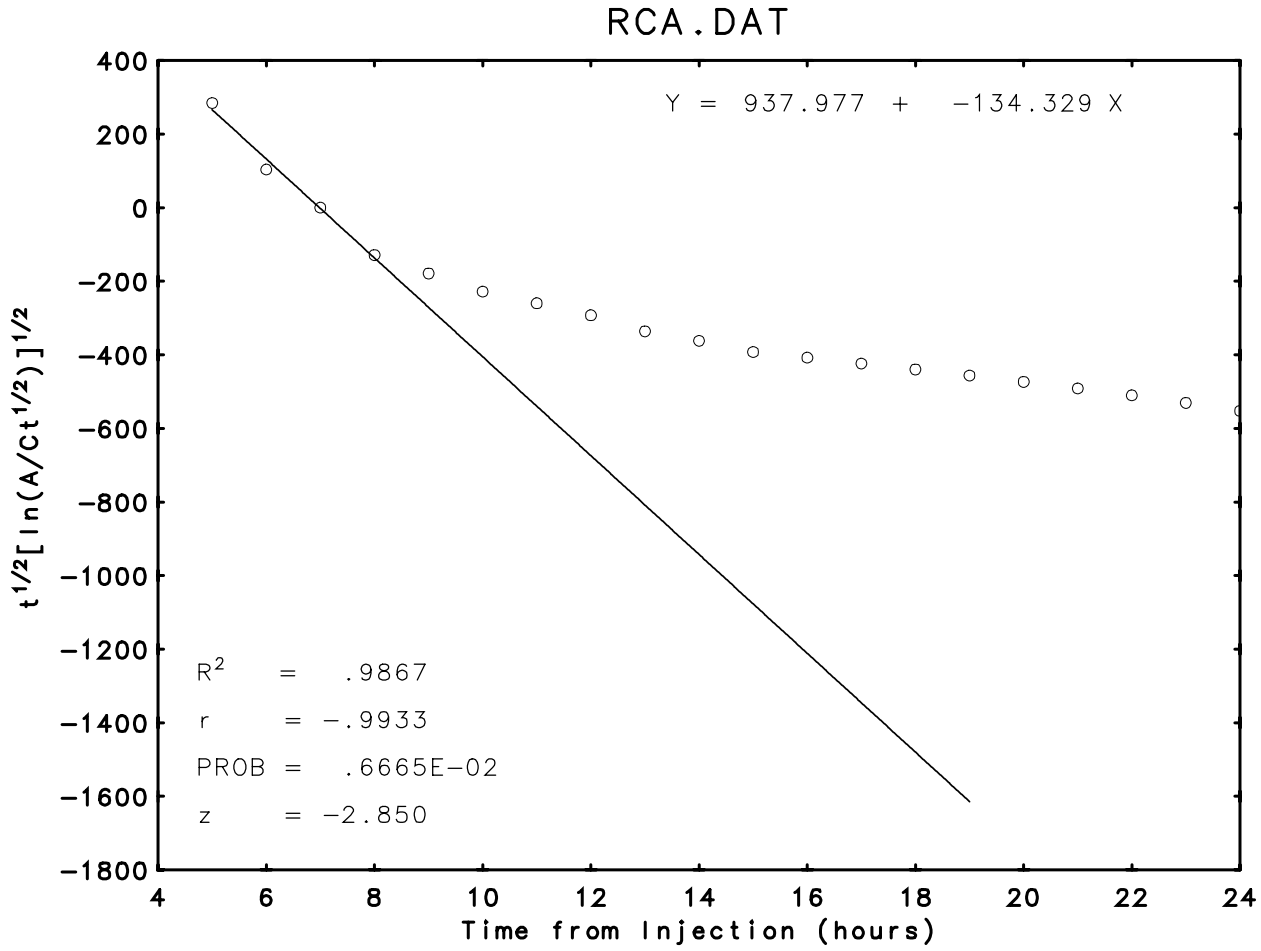

Figure 23. Plot and straight-line fit of the Chatwin parameter for the RCA.DAT sampling station data file.

```
**********************************************************************
**********************************************************************

          ------------------------------------

           Listing of output for:  RCA.DAT

          ------------------------------------

Limits to integration for the data file:RCA.DAT

 Lower integration limit                        .00000      hrs
 Upper integration limit                        24.000      hrs



The quantity of tracer recovered                1.7403      kg
                                                1740.3      g
                                                .17403E+07  mg
                                                .17403E+10  ug


Distance from input to outflow point            50.292      km
                                      (         165.00      ft)
Corrected for sinuosity = 1.50X


Time to leading edge (first arrival)            5.0000      hrs


Time to peak tracer concentration               7.0000      hrs
For a peak tracer concentration                 380.00      ug/L
```

Figure 24. Output file for the `RCA.DAT` sampling station data file.

```
The mean tracer transit time                    .36687       d
                                                8.804829     hrs
                                                528.2897000  min

Standard deviation for tracer time              .14560       d
                                                3.4945       hrs
                                                209.6686000  min


The mean tracer velocity                        137.0848000  m/d
                                                5.711866     m/hr
                                                0.15866E-02  m/s

Standard deviation for tracer velocity          19.330       m/d
                                                .80543       m/hr
                                                .22373E-03   m/s



Dispersion coefficient                          .71871E-03   m^2/s
Longitudinal dispersivity                       .45298       m


Peclet number                                   139.65
                                                Advection > Diffusion


The maximum tracer velocity                     241.4016000  m/d
                                                10.05840     m/hr
                                                .27940E-02   m/s
```

Figure 24. Output file for the `RCA.DAT` sampling station data file (continued).

```
Karst-conduit volume estimate                    .11.999     m^3

Karst-conduit cross-sectional area               .23858      m^2
Karst-conduit surface area                      35007.070    m^2
 Tracer sorption coefficient (conduit)          .51651E-01   m

Hydraulic head loss along conduit               .98203E-06   m
 Based on a friction factor                     .83435E-01


Estimated Reynolds number                       767.0682000
 Based on an estimated tube diameter            .55115       m
 and an hydraulic conductivity                  81662.       m/s


Estimated Froude number                         .77006E-03
 Based on an estimated hydraulic depth          .43288       m


Shear velocity                                  .28791E-03   m/s


Molecular mass transport parameters
 Estimated Schmidt number                       1140.026000
 Estimated Sherwood number                      122.374600
 Mass transfer coef. from wall to flow          .22203E-06   m/s
 Molecular diffusion layer thickness            4.5038       mm


Percent recovery of tracer injected             .6592        %
Accuracy index (0.0 = Perfect Recov.)           .9934
```

Figure 24. Output file for the `RCA.DAT` sampling station data file (continued).

```
**********************************************************************
**********************************************************************

     ------------------------------------------

       Listing of total estimates for:  rca.d

     ------------------------------------------

Total quantity of tracer recovered                  1.7403      kg
                                                    1740.3      g



Total aquifer volume estimate                       11.999      m^3

Total aquifer surface area estimate                 35007.070   m

Final tracer sorption coefficient                   .51651E-01  m


Percent recovery of tracer injected                 .6592       %
Accuracy index (0.0 = Perfect Recov.)               .9934
```

Figure 24. Output file for the `RCA.DAT` sampling station data file (continued).

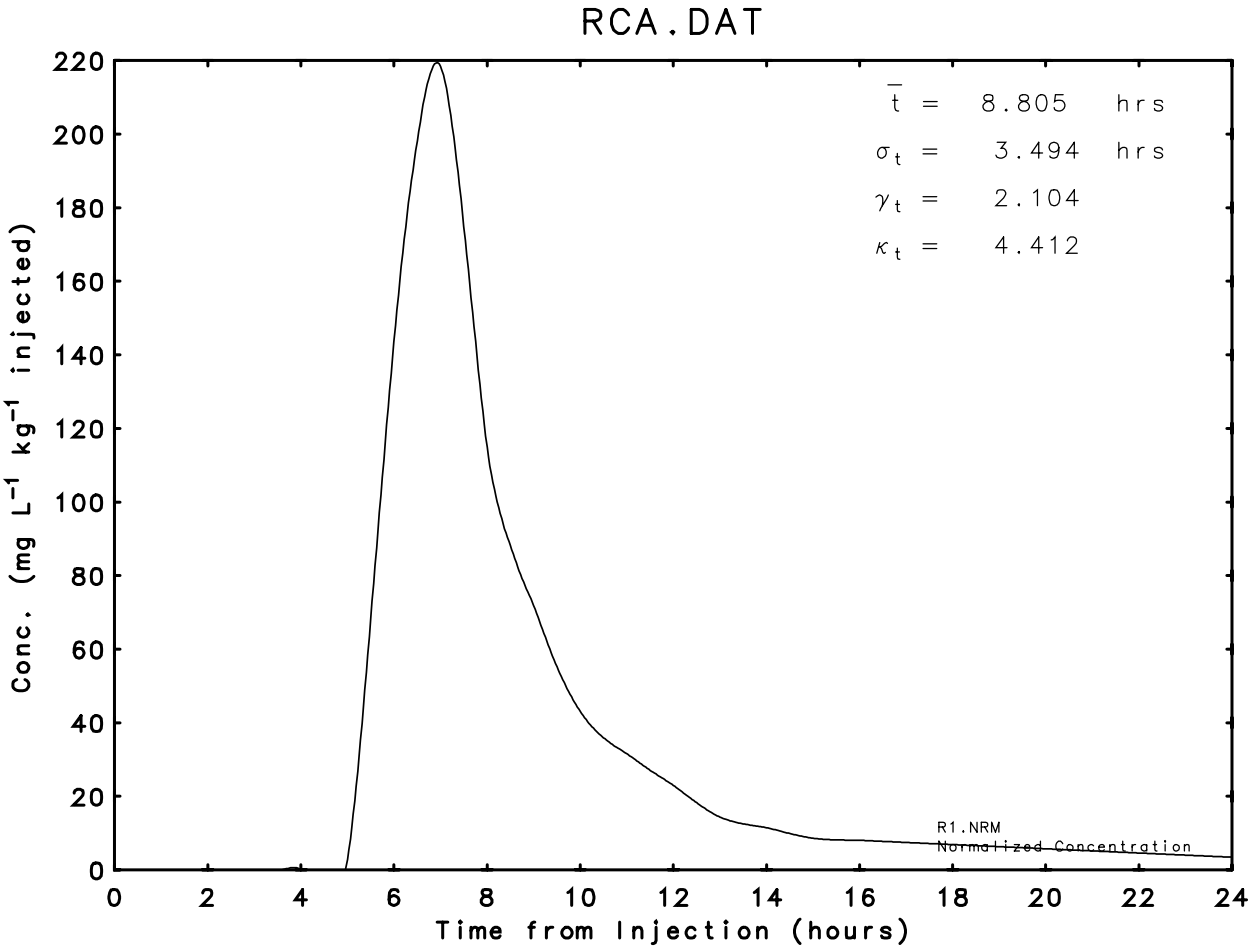

Figure 25. Normalized tracer concentration data for the RCA.DAT sampling station data file.

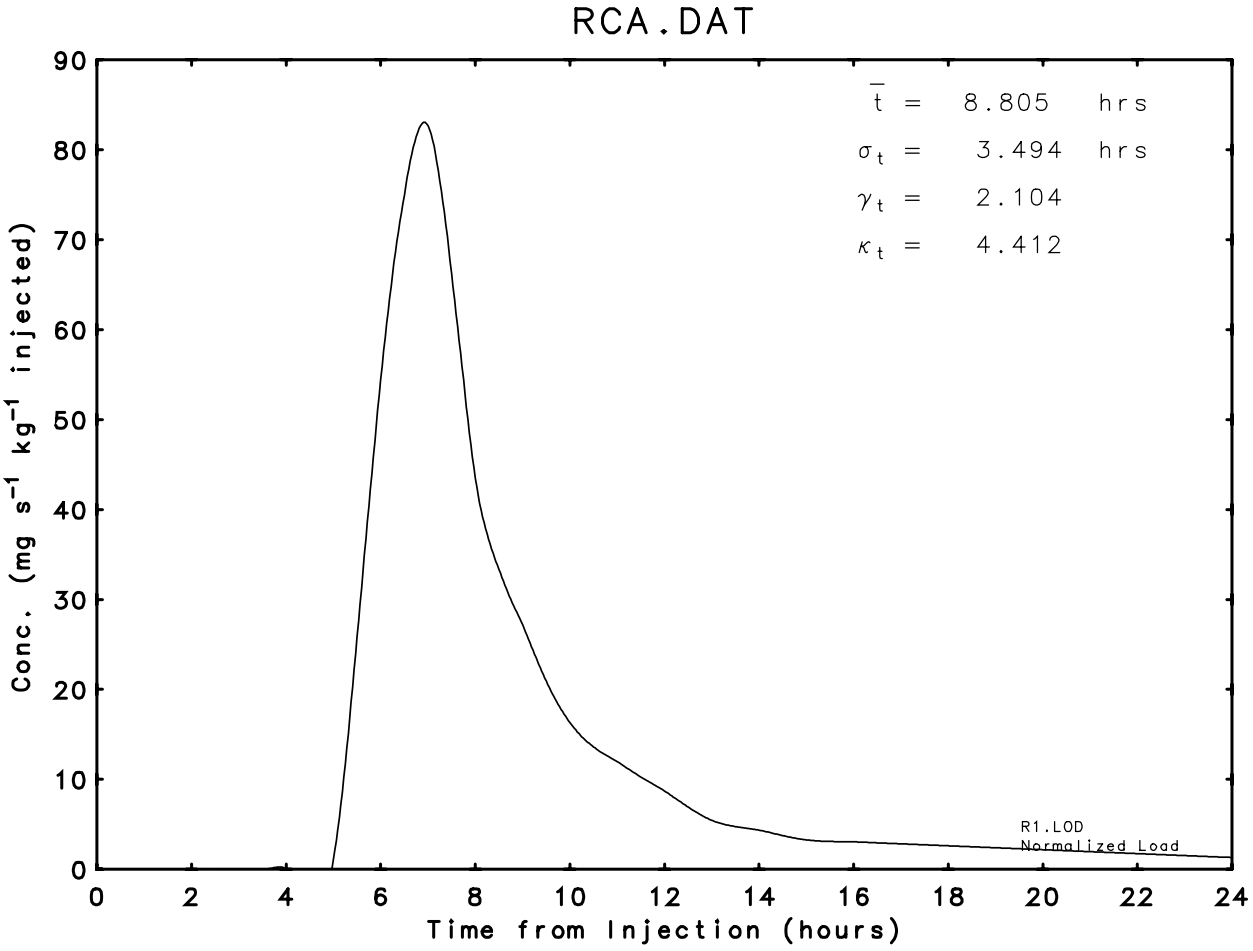

Figure 26. Normalized tracer load data for the RCA.DAT sampling station data file.

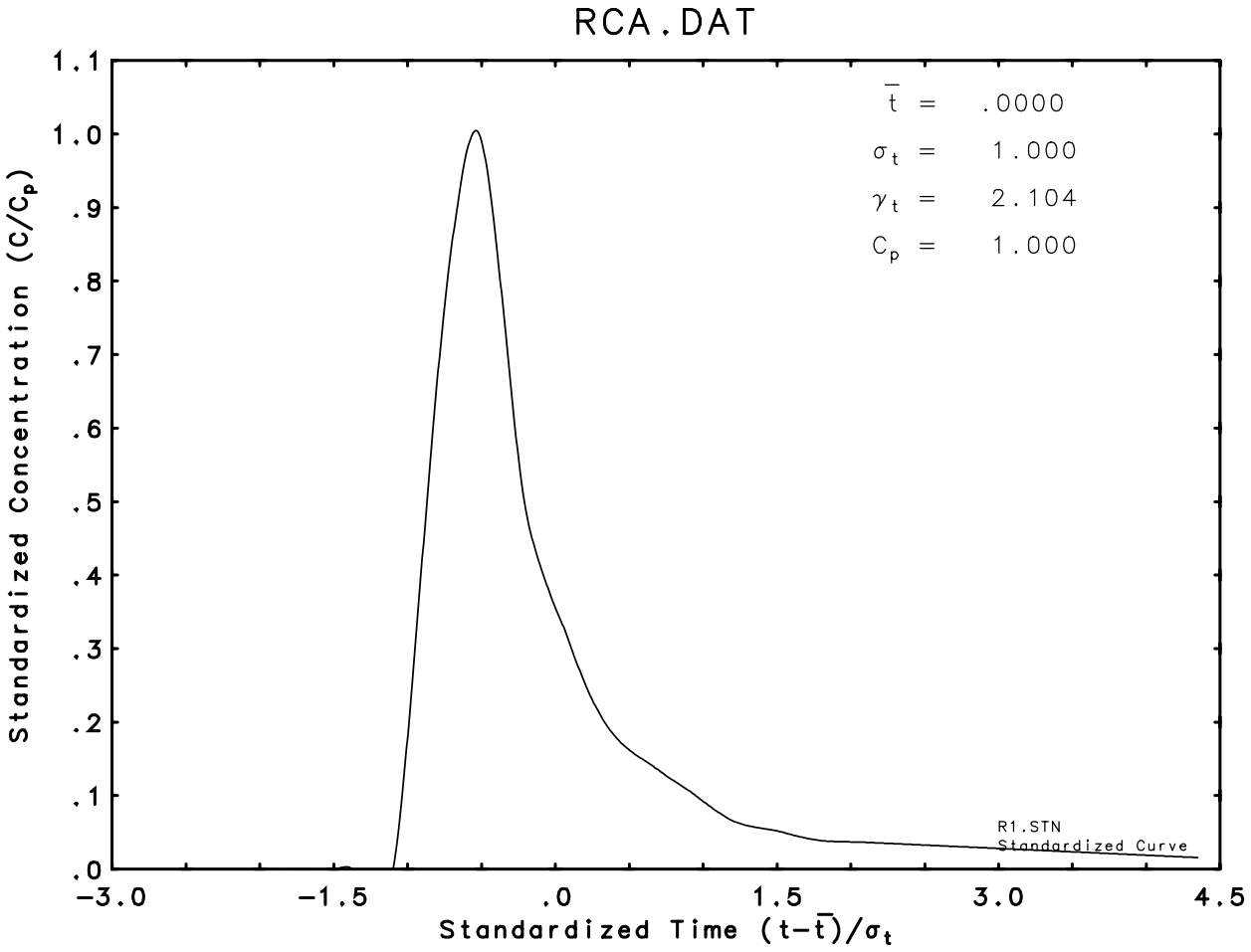

Figure 27. Standardized time-concentration data for the RCA.DAT sampling station data file.

7.3. ANALYSIS ASSESSMENT OF THE TWO EXAMPLE DATA FILES

From the two examples (ATKIN and RCA), it is apparent that QTRACER is not affected by variable discharges versus a constant discharge. QTRACER is also not affected by recovery at a spring versus recovery at a monitoring well.

It will be noted that the ATKIN data set resulted in nearly perfect mass recovery. Had the ATKIN data set been analyzed according to the description given in Section 4., the user would have noted that mass recovery was > 100%. The efficient integration algorithms used by QTRACER results in a more reliable mass balance.

QTRACER results for the RCA data set were quite similar to those presented in Section 4.1.1.. QTRACER performs equally well on less ideal sites (*e.g.*, TOPLITA).

7.3.1. Molecular Diffusion Layer Thickness

An estimate of the molecular diffusion layer thickness δ_m appears at the end of Figures 18 and 24. It is useful for understanding mass transfer from the walls of a karst conduit into the main flow stream. Estimation of δ_m may be achieved from (Dreybrodt, 1988, p. 172)

$$N_{sh} = D_C/\delta_m \tag{45}$$

where the Sherwood number N_{sh} for turbulent flow is obtained from (Dreybrodt, 1988, p. 172)

$$N_{sh} = 0.023 N_R^{0.83} N_{sc}^{1/3} \tag{46}$$

which is valid for $0.6 \leq N_{sc} \leq 2500$ and $2000 \leq N_R \leq 35000$. For laminar flow conditions N_{sh} may be estimated from

$$N_{sh} = 3.65 + \frac{0.668(D_C/x_s)N_R N_{sc}}{1 + 0.04[(D_C/x_s)N_R N_{sc}]^{0.67}} \tag{47}$$

A mass transfer coeficient k_f is obtained from the Sherwood number by using the relationship (Dreybrodt, 1988, p. 171)

$$N_{sh} = \frac{k_f D_C}{D_m} \tag{48}$$

where the molecular diffusivity is on the order of 10^{-9} m^2 s^{-1} (Neretnieks, 1993, p. 109).

The Schmidt number N_{sc} relates momentum and mass transfer. It is estimated by relating the molecular diffusivity of the tracer to the kinematic viscosity of the water according to the relationship

$$N_{sc} = \frac{\mu}{\rho D_m} \tag{49}$$

8. DATA INTERPOLATION AND EXTRAPOLATION EFFECTS

As explained in Section 5.1., QTRACER utilizes a very efficient data interpolation routine. The primary use of the data interpolation routine would be if the user believes that missing datapoints can be reasonably approximated by data interpolation. For example, if the user believes that unaltered tracer-breakthrough curves suggest that data aliasing may have occurred, then data interpolation may be able to confirm or deny if aliasing really has occurred.

8.1. COMPARISON OF ATKIN.DAT OUTPUT FILES

To illustrate the effect of data interpolation, data extrapolation, and the combined effect of data interpolation and extrapolation on a data set exhibiting good mass recovery, the ATKIN.DAT data set was subjected to each of these three algorithms. In some instances, the effect is fairly noticeable while in other instances there are no differences.

8.1.1. Interpolated ATKIN.DAT Tracer-Breakthrough Curve

Figure 28 depicts the interpolated tracer-breakthrough curve generated by QTRACER and analyzed by QTRACER. Note that discharge has an interpolated value for each time an interpolated tracer concentration value was created.

Graphically, the user will note that Figure 28 is more reasonable than Figure 16. The improvement is most evident at the peak, where the interpolated file more correctly matches the peak concentration datapoint. In Figure 16, the peak concentration is actually exceeded by the graphics line. However, the apparent inaccurate plotting is *NOT* reflected in the actual data analysis by QTRACER.

8.1.2. Interpolated ATKIN.DAT Chatwin Plot

Figure 29 depicts the interpolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

Some difference will be noted between Figure 29 and Figure 17, but not a significant difference. Interpolation results in more datapoints falling on the necessary straight line and the equation of the straight line has different values for the y intercept and slope. As such, a slightly different estimate for longitudinal dispersion will result.

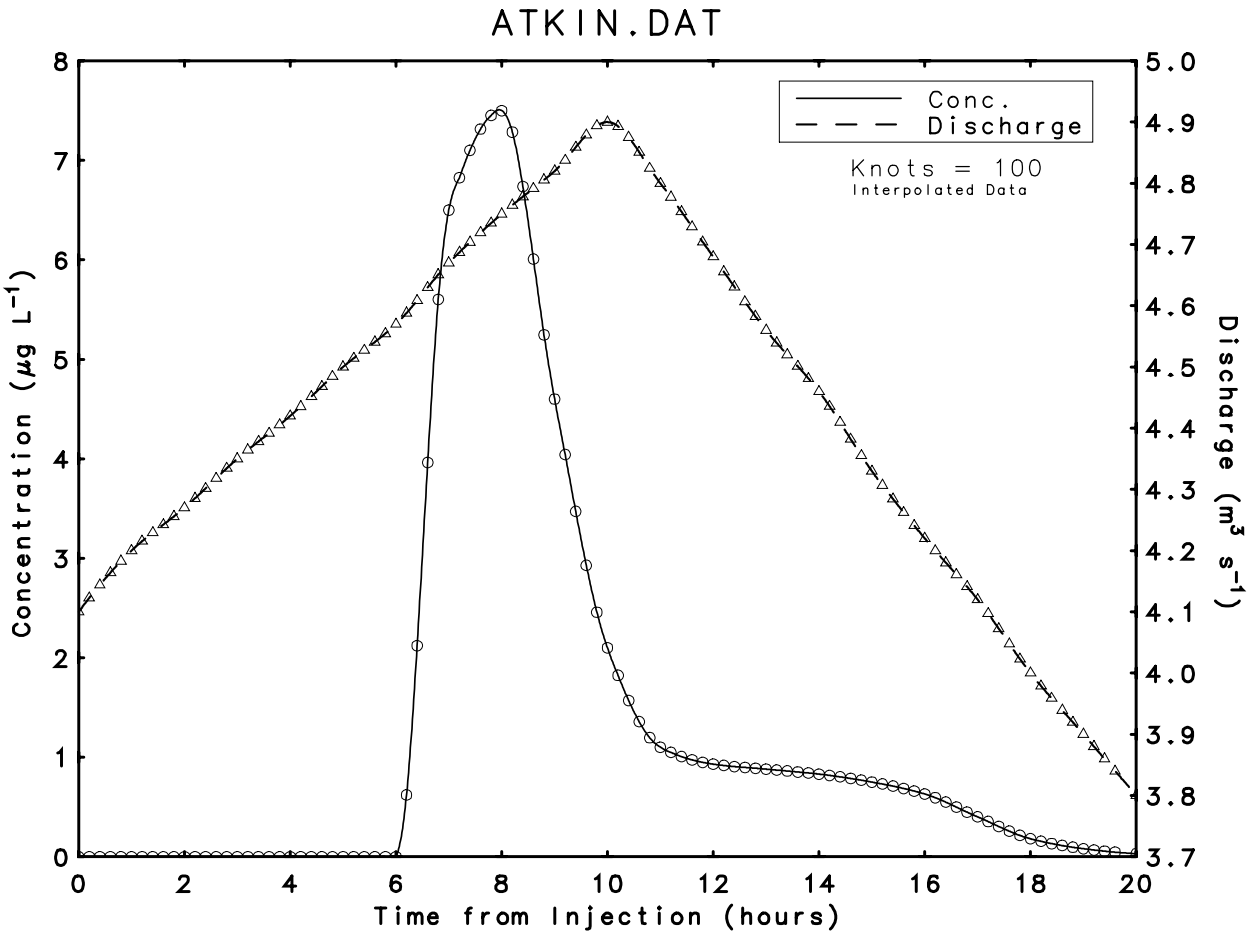

Figure 28. Interpolated curve for the ATKIN.DAT sampling station data file.

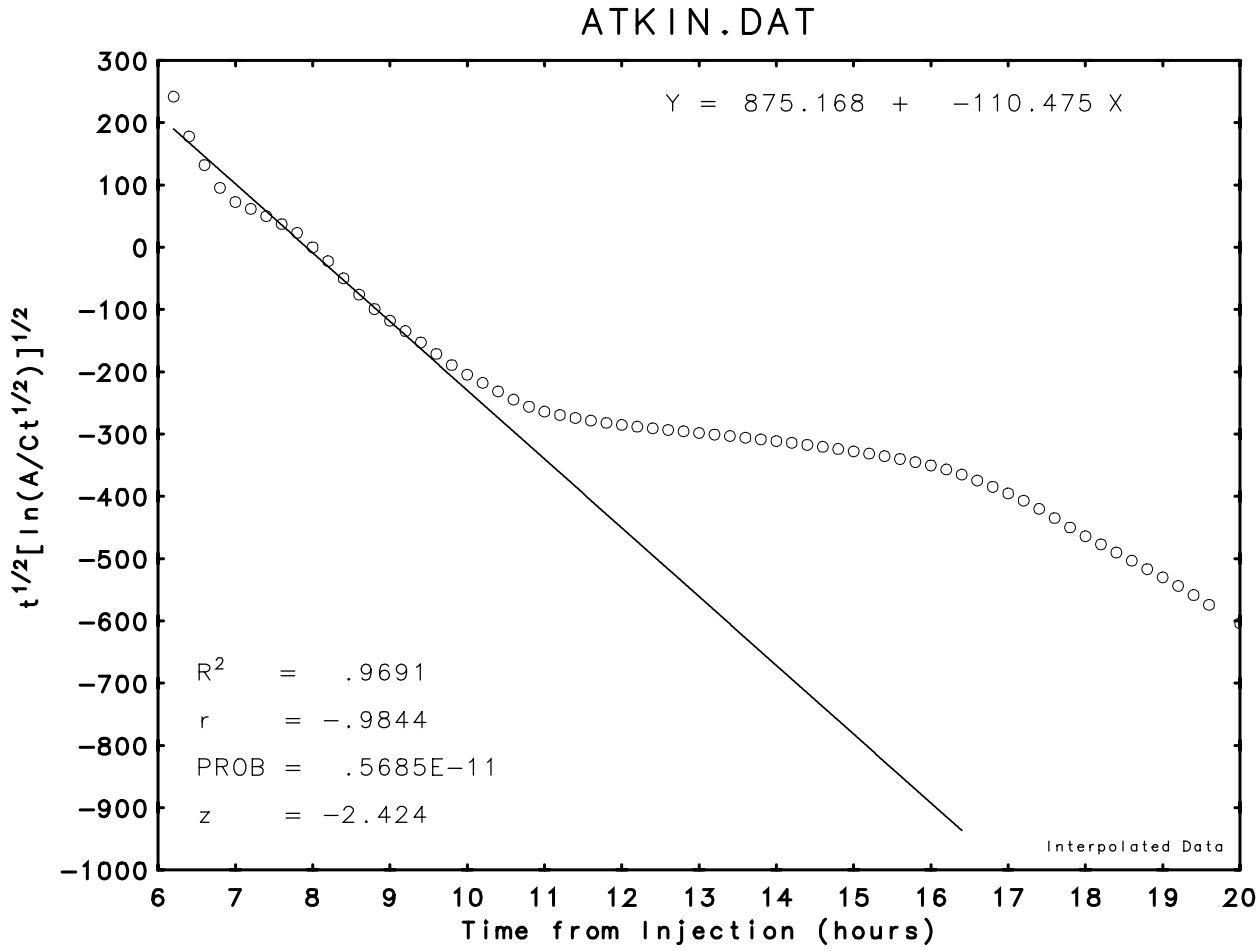

Figure 29. Interpolated data set for the Chatwin parameter for the ATKIN.DAT sampling station data file.

Table 6 compares the final analytical output for the unaltered tracer-breakthrough curve for the ATKIN.DAT data set, the interpolated ATKIN.DAT data set, and the Interpolated-extrapolated ATKIN.DAT data set. Note how each file's results are closely matched with the others.

8.1.3. Extrapolated ATKIN.DAT Tracer-Breakthrough Curve

Figure 30 depicts the extrapolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has an interpolated value for each time an extrapolated tracer concentration value was created.

Graphically, the user will note that the tracer-breakthrough curve shown in Figure 30 appears relatively unchanged from Figure 16. The only apparent difference is that the elapsed tracer travel time has been extended from 20 hours to > 22 hours and that one additional datapoint (total data = 22) has been included.

More obvious is the effect of data extrapolation on the discharge curve when data extrapolation routines `1` (exponential decay) and `3` (statistical fit) are employed (`3` = statistical fit for Figure 30). Extrapolation routine `2` (piecewise cubic Hermite) uses the shape of the entire existing data curve to determine the "most reasonable" extrapolation datapoint possible for the extrapolated discharge.

Extrapolation routines `1` and `3`, however, have no mathematical basis for consideration. For example, there is no reason to assume that discharge will behave as an exponential decay function, so extrapolation routine `1 = exponential decay` would make no physical sense. Therefore, when extrapolation routines `1` or `3` are requested and a variable discharge was measured, QTRACER will automatically extend the discharge curve in the opposite vertical direction (along the y axis) to one-half its previous range. It is up to the user to decide on its reasonableness.

8.1.4. Extrapolated ATKIN.DAT Chatwin Plot

Figure 31 depicts the extrapolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the straight-line fit, the equation for the straight-line, and the relevant statistics describing the straight-line fit generated by QTRACER are identical to Figure 17. Data extrapolation had no effect on the Chatwin method analysis because original sample had resulted in nearly "complete" tracer recovery.

Table 6. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for ATKIN.DAT sampling station.

Parameter	ATKIN.DAT (unaltered)	ATKIN.DAT (interpolated)	ATKIN.DAT[1] (extrapolated)	ATKIN.DAT[2] (inter./extra.)
Tracer Mass Recovered, g	4.48×10^{2}	4.48×10^{2}	4.48×10^{2}	4.48×10^{2}
Percent Mass Recovered	9.96×10^{1}	9.95×10^{1}	9.96×10^{1}	9.96×10^{1}
Accuracy Index	4.48×10^{-3}	4.75×10^{-3}	3.67×10^{-3}	3.80×10^{-3}
Initial Tracer Breakthrough, h	7.00×10^{0}	6.20×10^{0}	7.00×10^{0}	6.10×10^{0}
Time to Peak Concentration, h	8.00×10^{0}	8.00×10^{0}	8.00×10^{0}	8.00×10^{0}
Mean Tracer Residence Time, h	9.27×10^{0}	9.26×10^{0}	9.28×10^{0}	9.27×10^{0}
Elapsed Tracer Travel Time, h	2.00×10^{1}	2.00×10^{1}	2.26×10^{1}	2.32×10^{1}
Maximum Tracer Flow Velocity, m s^{-1}	1.07×10^{-1}	1.21×10^{-1}	1.07×10^{-1}	1.23×10^{-1}
Peak Tracer Flow Velocity, m s^{-1}	9.38×10^{-2}	9.38×10^{-2}	9.38×10^{-2}	9.38×10^{-2}
Mean Tracer Flow Velocity, m s^{-1}	8.09×10^{-2}	8.10×10^{-2}	8.08×10^{-2}	8.09×10^{-2}
Shear Velocity, m s^{-1}	1.70×10^{-2}	1.70×10^{-2}	1.70×10^{-2}	1.70×10^{-2}
Longitudinal Dispersion, m^2 s^{-1}	3.26×10^{0}	2.38×10^{0}	3.26×10^{0}	2.13×10^{0}
Hydraulic Head Loss, m	1.20×10^{-2}	1.21×10^{-2}	1.20×10^{-2}	1.20×10^{-2}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a statistical straight line fit.
[2]Extrapolated using a cubic Hermite function.

Table 6. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for ATKIN.DAT sampling station (cont.).

Parameter	ATKIN.DAT (unaltered)	ATKIN.DAT (interpolated)	ATKIN.DAT[1] (extrapolated)	ATKIN.DAT[2] (inter./extra.)
Conduit Volume, m^3	1.49×10^5	1.49×10^5	1.50×10^3	1.50×10^3
Conduit Cross-Sectional Area, m^2	5.53×10^1	5.53×10^1	5.54×10^1	5.54×10^1
Conduit Surface Area, m^2	5.16×10^7	5.16×10^7	5.15×10^7	5.15×10^7
Tracer Sorption Coefficient, m	1.31×10^{-5}	1.38×10^{-5}	1.07×10^{-5}	1.11×10^{-5}
Conduit Diameter, m	8.39×10^0	8.40×10^0	8.40×10^0	8.40×10^0
Hydraulic Depth, m	6.59×10^0	6.59×10^0	6.60×10^0	6.59×10^0
Friction Factor	1.12×10^{-1}	1.12×10^{-1}	1.12×10^{-1}	1.12×10^{-1}
Laminar Flow Sublayer, m	1.38×10^{-3}	1.38×10^{-3}	1.38×10^{-3}	1.38×10^{-3}
Reynolds Number	5.96×10^5	5.96×10^5	5.95×10^5	5.96×10^5
Froude Number	1.01×10^{-2}	1.01×10^{-2}	1.01×10^{-2}	1.01×10^{-2}
Peclet Number	7.77×10^1	1.06×10^2	7.77×10^1	1.19×10^2
Schmidt Number	1.14×10^3	1.14×10^3	1.14×10^3	1.14×10^3
Sherwood Number	1.49×10^4	1.49×10^4	1.49×10^4	1.49×10^4
Mass Transfer Coefficient, m s^{-1}	1.78×10^{-6}	1.78×10^{-6}	1.78×10^{-6}	1.78×10^{-2}
Molecular diffusion layer, m	5.62×10^{-4}	5.62×10^{-4}	5.62×10^{-4}	5.63×10^{-4}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a statistical straight line fit.
[2]Extrapolated using a cubic Hermite function.

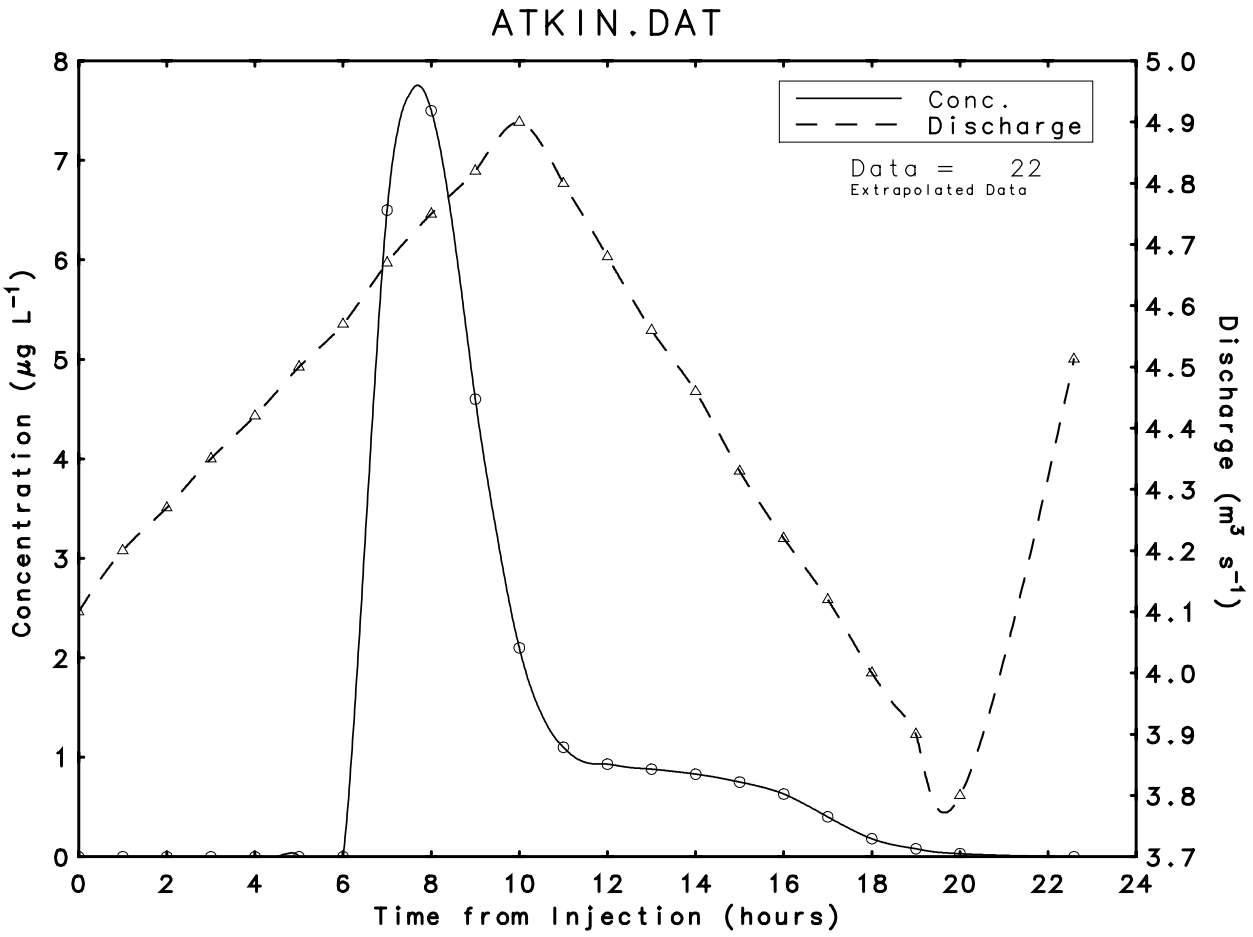

Figure 30. Extrapolated curve for the ATKIN.DAT sampling station data file.

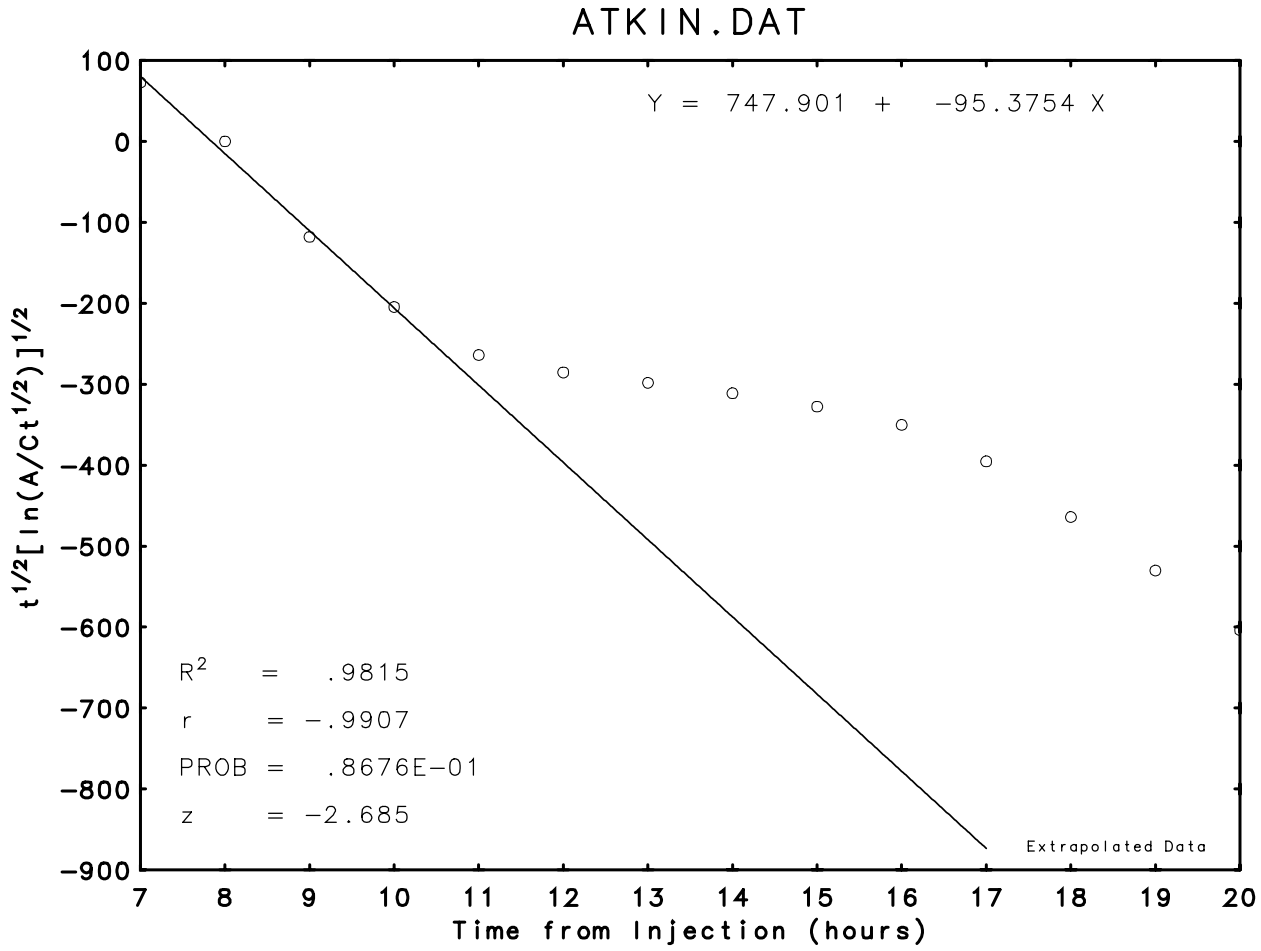

Figure 31. Extrapolated data set for the Chatwin parameter for the ATKIN.DAT sampling station data file.

8.2. INTERPOLATED-EXTRAPOLATED ATKIN.DAT DATA

Figures 32 and 33 illustrates how the interpolation and extrapolation routines provided in QTRACER can be used to in tracer-breakthrough curve analyses. Table 6 illustrates that there are no significant differences in any of the analyses provided by QTRACER for the ATKIN.DAT data set.

A more erratic tracer-breakthrough curve, or one that was ended leaving a significant mass of tracer in the system, would result in large differences when data interpolation and/or extrapolation is employed. The user should note that when data extrapolation is employed without data interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured datapoint to the extrapolated datapoint). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER will develop a smooth curve between all provided datapoints regardless of tracer-breakthrough curve appearance.

8.3. COMPARISON OF RCA.DAT OUTPUT FILES

To further illustrate the effect of data interpolation, data extrapolation, and the combined effects of data interpolation and extrapolation on a data set exhibiting poor mass recovery, the RCA.DAT data set was subjected to each of these three algorithms. In some instances, the effect is fairly noticeable, while in other instances there are no differences.

8.3.1. Interpolated RCA.DAT Tracer-Breakthrough Curve

Figure 34 depicts the interpolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has no interpolated value. This is because discharge was considered a constant, so there are no data to interpolate.

Graphically, the user will note that Figure 34 is little changed from the curve shown in Figure 22. The slight improvement is most evident at the peak, where the interpolated file more correctly matches the peak concentration datapoint. In Figure 22, the graphics line slightly exceeds the time to peak concentration. However, the apparent inaccurate plotting is *NOT* reflected in the actual data analysis by QTRACER.

8.3.2. Interpolated RCA.DAT Chatwin Plot

Figure 35 depicts the interpolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the equation

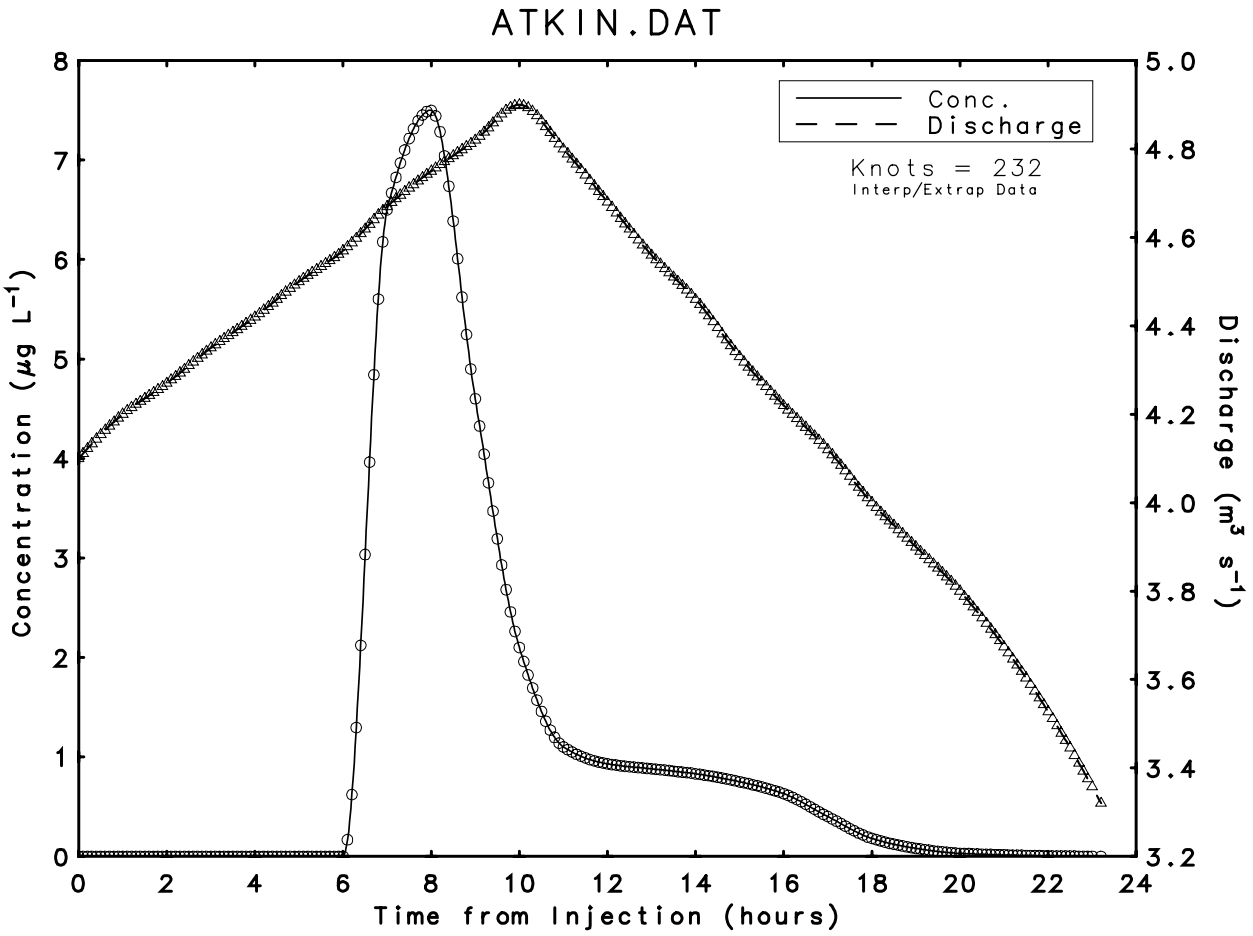

Figure 32. Interpolated and extrapolated data set for the ATKIN.DAT sampling station data file.

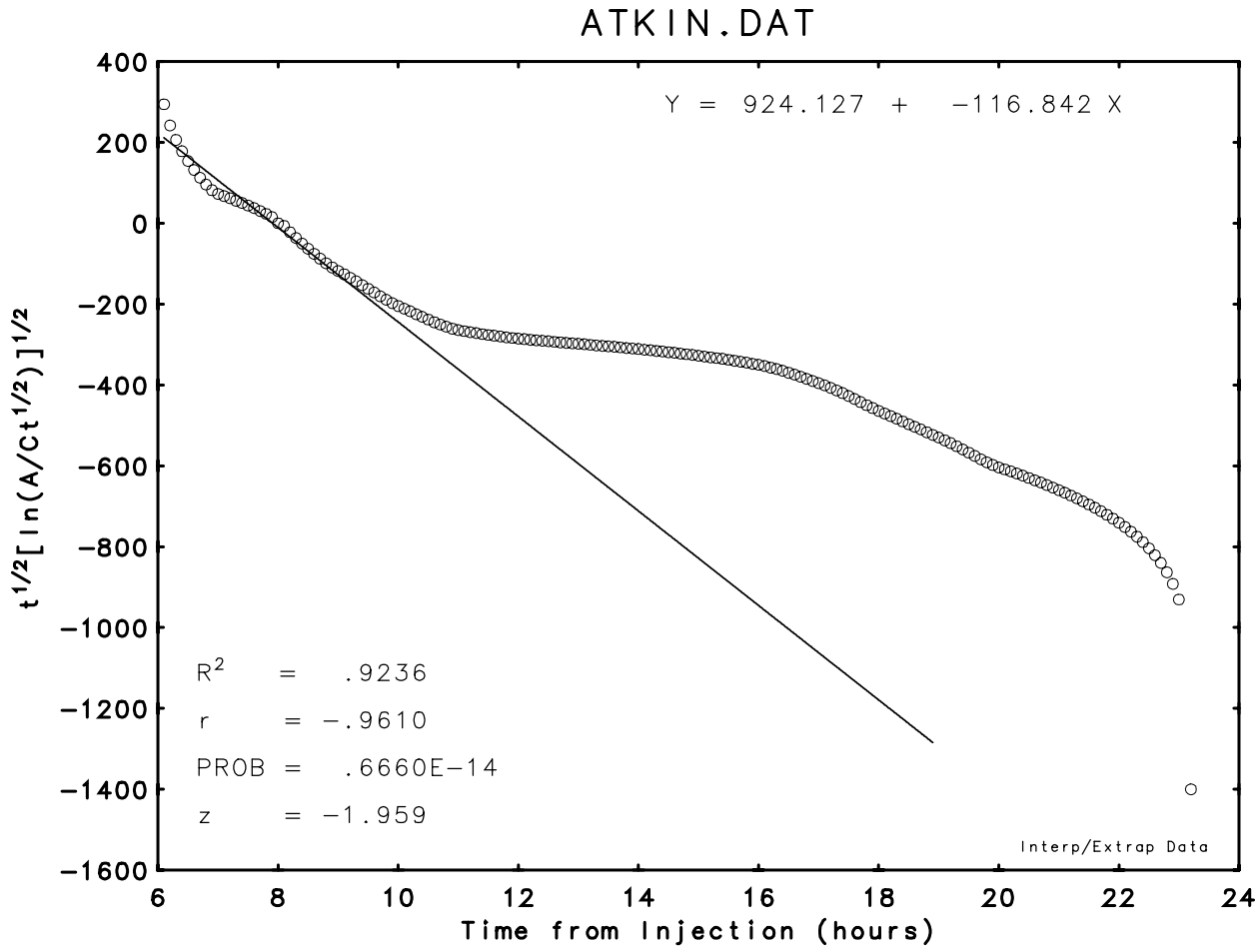

Figure 33. Interpolated and extrapolated data for the Chatwin parameter for ATKIN.DAT sampling station data file.

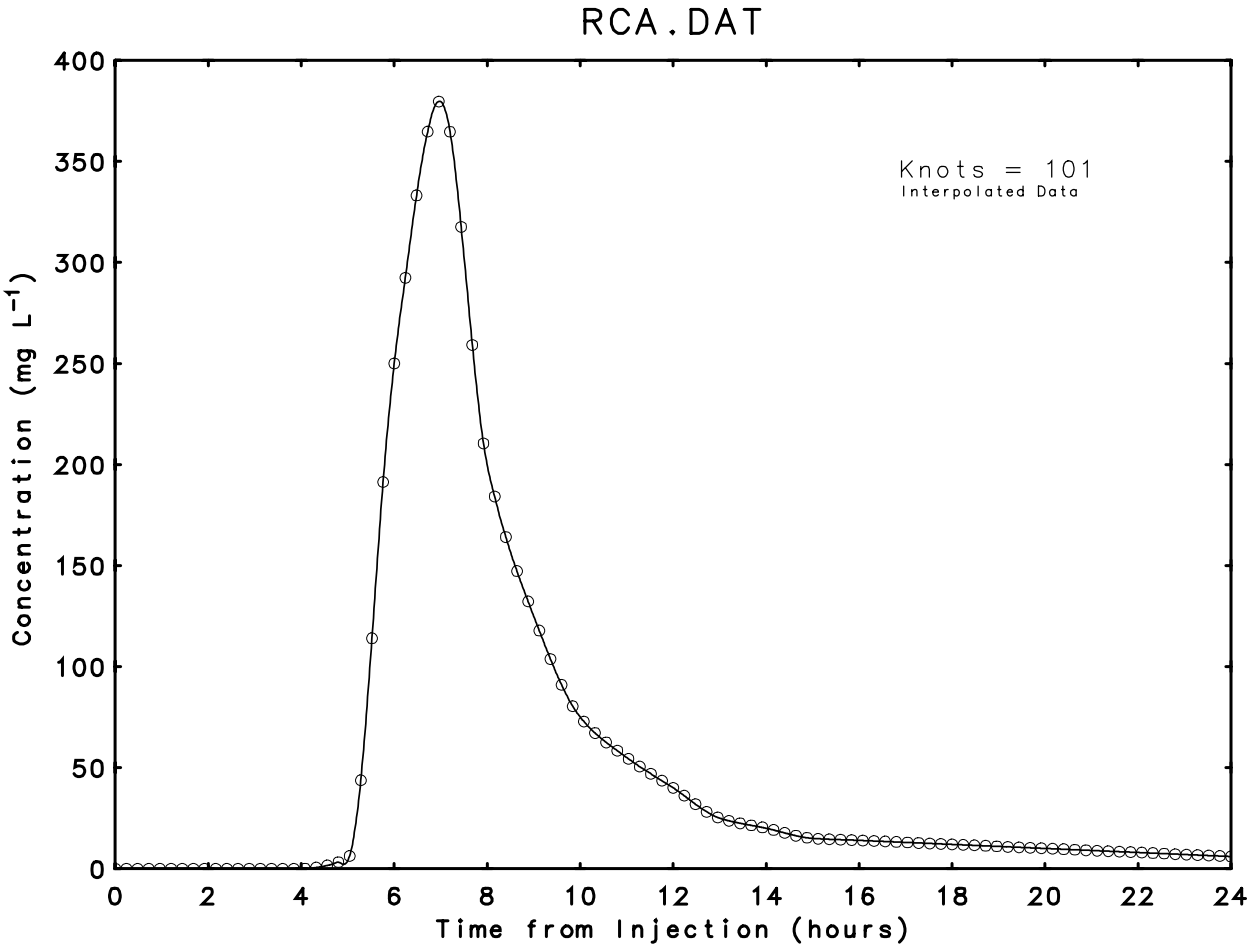

Figure 34. Interpolated curve for the RCA.DAT sampling station data file.

for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

Some difference will be noted between Figure 35 and Figure 23, but not a greatly significant difference. Interpolation results in more datapoints falling on the necessary straight line, and the equation of the straight line has different values for the y intercept and slope. As such, a slightly different estimate for longitudinal dispersion will result.

Table 7 compares the final analytical output for the unaltered tracer-breakthrough curve for the RCA.DAT data set, the interpolated RCA.DAT data set, and the interpolated-extrapolated RCA.DAT data set. Note how each file's results are closely matched with the others.

8.3.3. Extrapolated RCA.DAT Tracer-Breakthrough Curve

Figure 36 depicts the extrapolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has no extrapolated value because discharge was constant.

Graphically, the user will note that Figure 36 is more reasonable than Figure 22. The improvement is most evident at the elapsed time of travel. In Figure 22, the elapsed time of travel (24 hours) is reflected in a cessation of sample collection prior to "complete" tracer recovery. However, Figure 36 suggests nearly "complete" tracer recovery at > 30 hours.

8.3.4. Extrapolated RCA.DAT Chatwin Plot

Figure 37 depicts the extrapolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the straight-line fit, equation for the straight-line, and relevant statistics describing the straight-line fit generated by QTRACER are slightly different from the results shown in Figure 23.

The obvious differences in between Figure 37 and Figure 23 are a result of not having continued actual data collection until near "complete" tracer recovery. Because sampling ceased before adequate tracer recovery, data extrapolation exerts considerable influence on the Chatwin analysis; in this instance, a less good straight-line fit to the data.

8.4. INTERPOLATED-EXTRAPOLATED RCA.DAT DATA

Figures 38 and 39 illustrate how the interpolation and extrapolation routines provided in QTRACER can be used in tracer-breakthrough curve analyses. Table 7 illustrates that there are no significant differences in any of the analyses provided by QTRACER for the RCA.DAT data set.

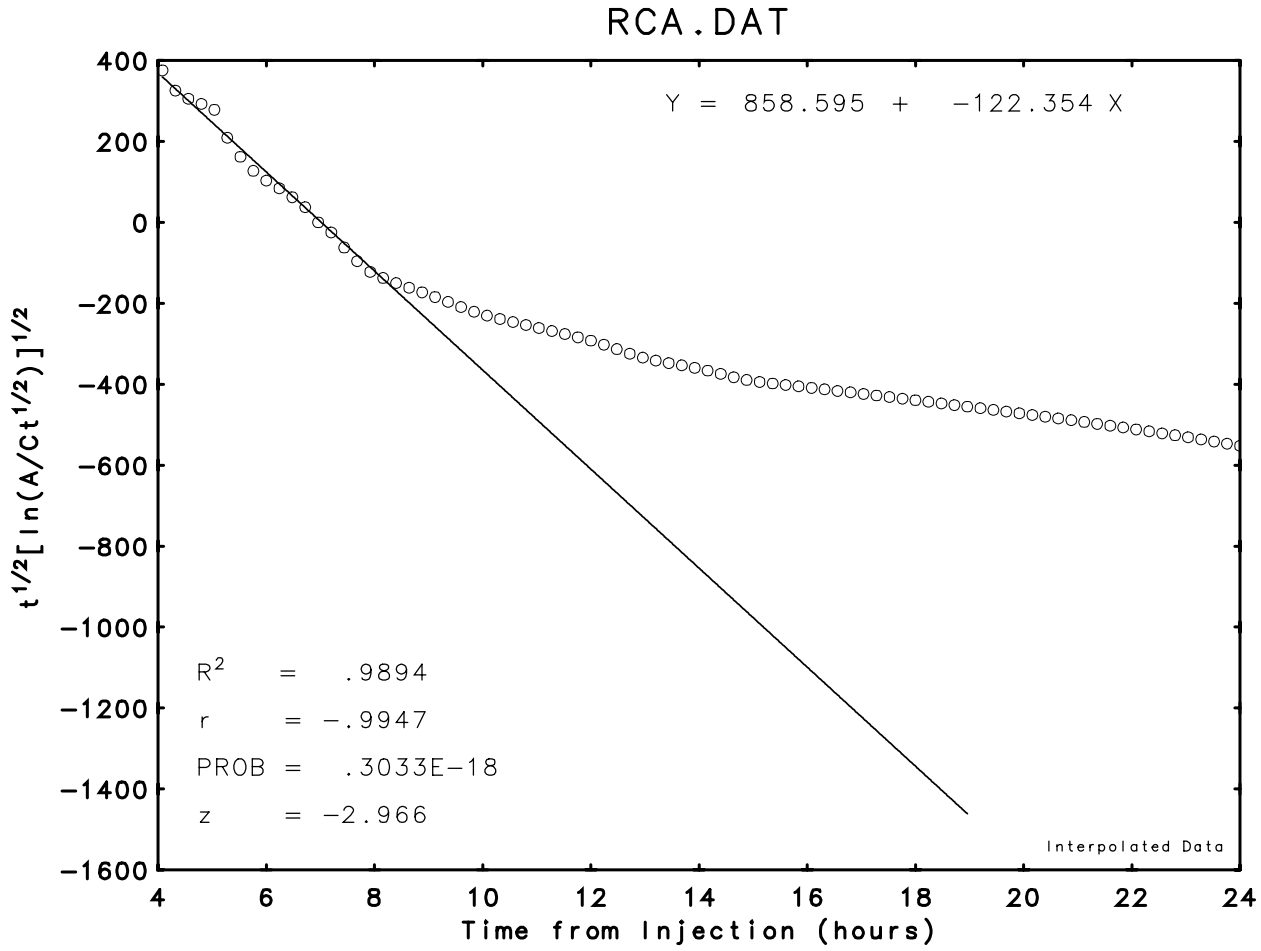

Figure 35. Interpolated data set for the Chatwin parameter for the RCA.DAT sampling station data file.

Table 7. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for RCA.DAT sampling station.

Parameter	RCA.DAT (unaltered)	RCA.DAT (interpolated)	RCA.DAT[1] (extrapolated)	RCA.DAT[2] (inter./extra.)
Tracer Mass Recovered, g	1.74×10^{3}	1.74×10^{3}	1.77×10^{3}	1.77×10^{3}
Percent Mass Recovered	6.59×10^{-1}	6.59×10^{-1}	6.70×10^{-1}	6.71×10^{1}
Accuracy Index	9.93×10^{-1}	9.93×10^{-1}	9.93×10^{-1}	9.93×10^{-1}
Initial Tracer Breakthrough, h	5.00×10^{0}	4.08×10^{0}	5.00×10^{0}	4.08×10^{0}
Time to Peak Concentration, h	7.00×10^{0}	6.96×10^{0}	7.00×10^{0}	6.96×10^{0}
Mean Tracer Residence Time, h	8.81×10^{0}	8.80×10^{0}	9.10×10^{0}	9.15×10^{0}
Elapsed Tracer Travel Time, h	2.40×10^{1}	2.40×10^{1}	3.17×10^{1}	5.20×10^{1}
Maximum Tracer Flow Velocity, m s^{-1}	2.79×10^{-3}	3.42×10^{-3}	2.79×10^{-3}	3.42×10^{-3}
Peak Tracer Flow Velocity, m s^{-1}	2.00×10^{-3}	2.01×10^{-3}	2.00×10^{-3}	2.01×10^{-3}
Mean Tracer Flow Velocity, m s^{-1}	1.59×10^{-3}	1.59×10^{-3}	1.54×10^{-3}	1.53×10^{-3}
Shear Velocity, m s^{-1}	2.88×10^{-4}	2.88×10^{-4}	2.81×10^{-4}	2.80×10^{-4}
Longitudinal Dispersion, m^2 s^{-1}	7.19×10^{-4}	8.58×10^{-4}	9.24×10^{-4}	9.32×10^{-4}
Hydraulic Head Loss, m	9.82×10^{-7}	9.83×10^{-7}	9.20×10^{-7}	9.10×10^{-7}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a cubic Hermite function.
[2]Extrapolated using an exponential decay function.

Table 7. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for RCA.DAT sampling station (cont.).

Parameter	RCA.DAT (unaltered)	RCA.DAT (interpolated)	RCA.DAT[1] (extrapolated)	RCA.DAT[2] (inter./extra.)
Conduit Volume, m^3	1.20×10^1	1.20×10^1	1.24×10^1	1.25×10^1
Conduit Cross-Sectional Area, m^2	2.39×10^{-1}	2.39×10^{-1}	2.47×10^{-1}	2.48×10^{-1}
Conduit Surface Area, m^2	3.50×10^4	3.50×10^4	3.47×10^4	3.47×10^4
Tracer Sorption Coefficient, m	5.17×10^{-2}	5.16×10^{-2}	5.29×10^{-2}	5.32×10^{-2}
Conduit Diameter, m	5.51×10^{-1}	5.51×10^{-1}	5.60×10^{-1}	5.62×10^{-1}
Friction Factor	8.34×10^{-2}	8.34×10^{-2}	8.48×10^{-2}	8.50×10^{-2}
Laminar Hydraulic Conductivity, m s^{-1}	8.17×10^4	8.16×10^4	8.44×10^4	8.48×10^4
Reynolds Number	7.67×10^2	7.67×10^2	7.55×10^2	7.53×10^2
Froude Number	7.70×10^{-4}	7.71×10^{-4}	7.40×10^{-4}	7.34×10^{-4}
Peclet Number	1.40×10^2	1.18×10^2	1.09×10^2	1.08×10^2
Schmidt Number	1.14×10^3	1.14×10^3	1.14×10^3	1.14×10^3
Sherwood Number	1.22×10^2	1.22×10^2	1.22×10^2	1.22×10^2
Mass Transfer Coefficient, m s^{-1}	2.22×10^{-7}	2.22×10^{-7}	2.19×10^{-7}	2.18×10^{-2}
Molecular diffusion layer, m	4.50×10^{-3}	4.50×10^{-3}	4.58×10^{-3}	4.59×10^{-3}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a cubic Hermite function.
[2]Extrapolated using an exponential decay function.

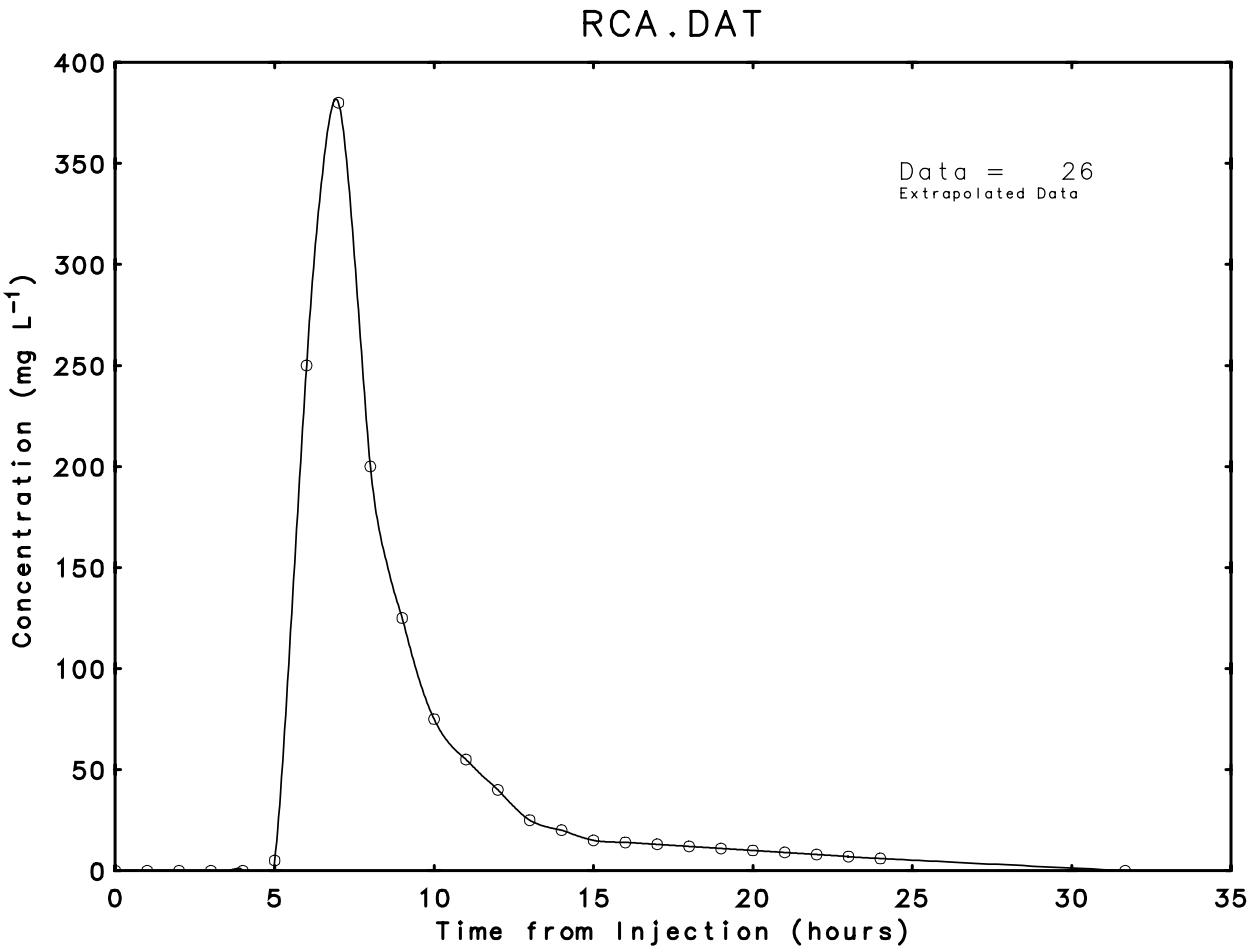

Figure 36. Extrapolated curve for the RCA.DAT sampling station data file.

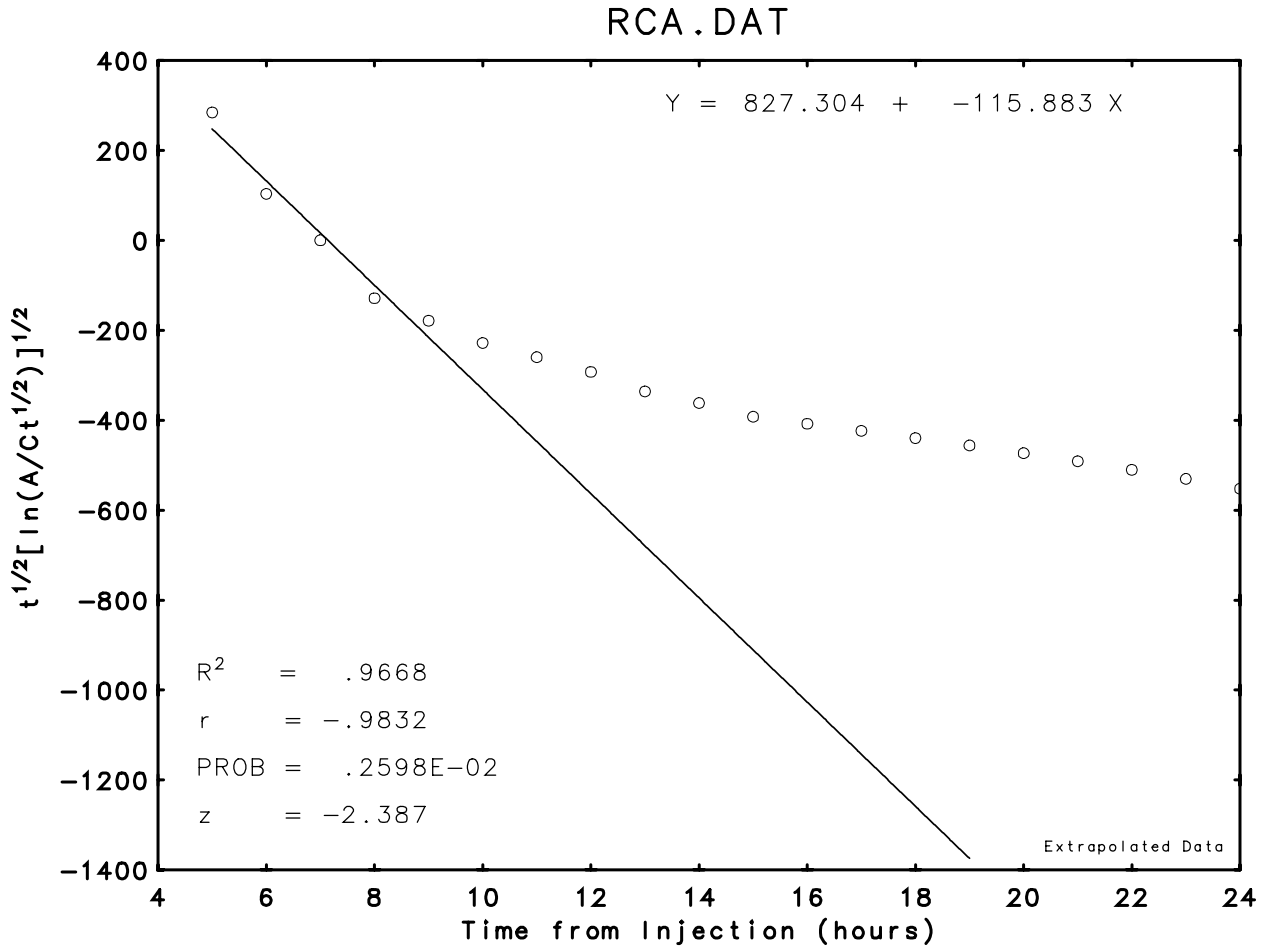

Figure 37. Extrapolated data set for the Chatwin parameter for the RCA.DAT sampling station data file.

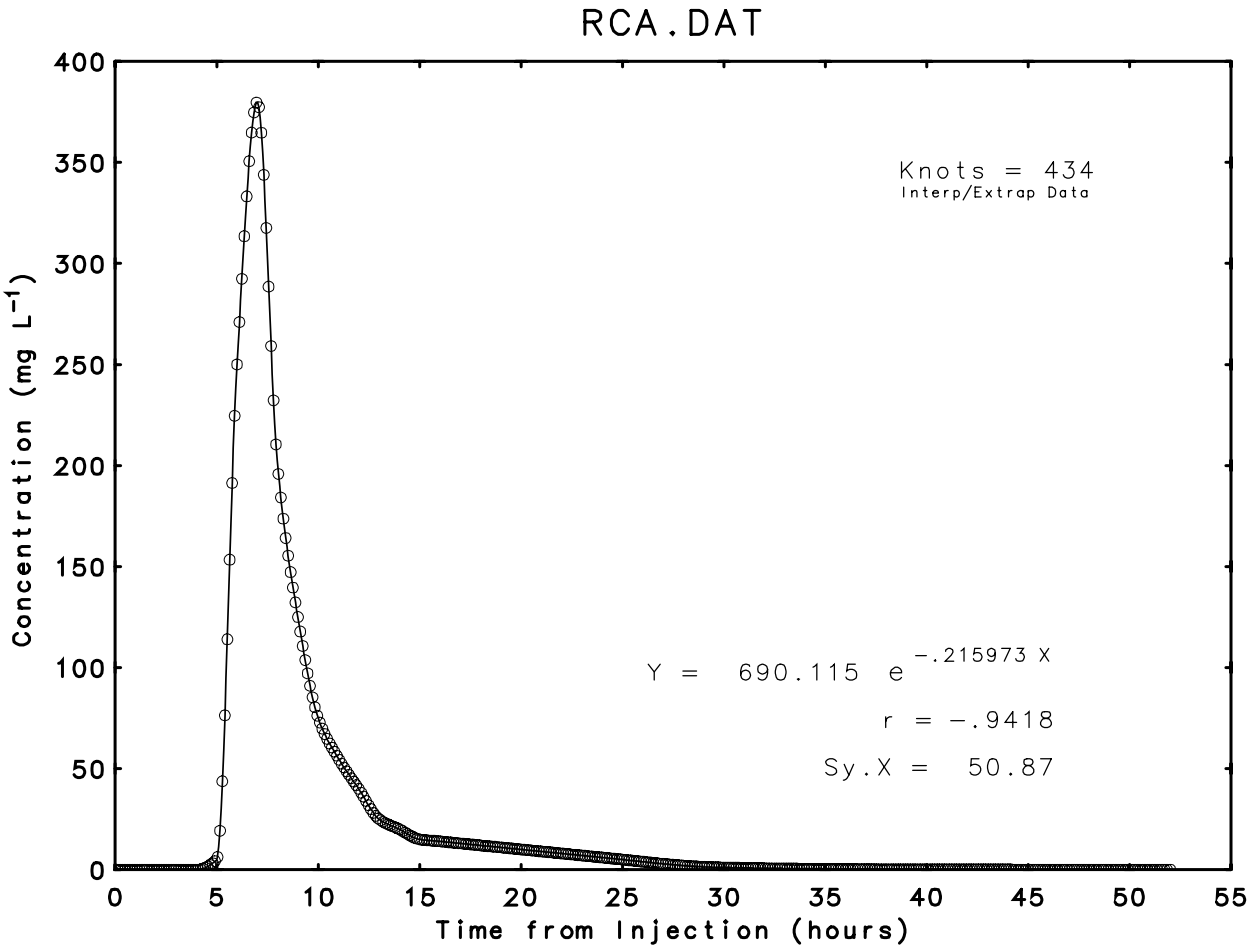

Figure 38. Interpolated and extrapolated data set for the RCA.DAT sampling station data file.

The user will note in Figures 38 that the exponential decay equation

$$y = 690.115\mathrm{e}^{-0.21597x} \tag{50}$$

has been produced along with the correlation coefficient r (-0.9418) and the standard error of the estimated fit (50.87). QTRACER provides this information to the user to assist in assessing the effect of an exponential decay on a tracer-breakthrough curve. It will be noted that whereas extrapolation methods `2` (piecewise cubic Hermite) and `3` (statistical method) produce a single extrapolated point, method `1` (exponential decay) produces five additional datapoints and thus has a great deal more influence on the final results.

Exponential decay extrapolation has more influence because the integration routine employed by QTRACER is forced to conform to the shape of the exponentially decaying curve. It is therefore incumbent upon the user to determine the appropriateness of using an exponential decay model for extrapolation. For example, applying an exponential decay for extrapolation to the ATKIN.DAT data set results in tracer mass recovery that is greater than what was injected. Clearly this is an impossibility that suggests major field errors, laboratory errors, numerical errors, or some combination of all three.

A more erratic tracer-breakthrough curve or one that was ended leaving a significant mass of tracer in the system would result in large differences when data interpolation and/or extrapolation is employed. The user should note that when data extrapolation is employed without data interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured datapoint to the extrapolated datapoint). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER will develop a smooth curve between all provided datapoints regardless of tracer-breakthrough curve appearance.

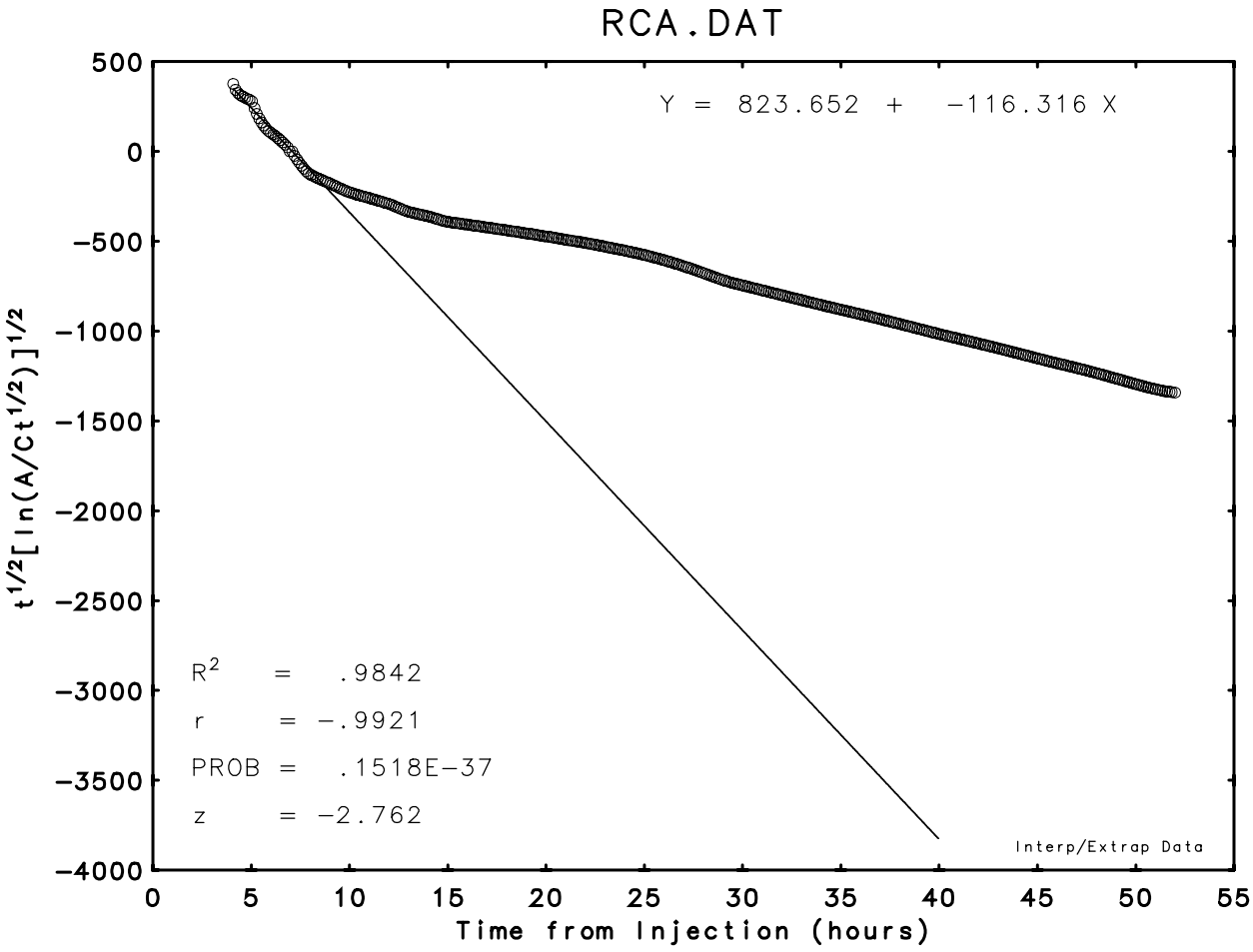

Figure 39. Interpolated and extrapolated data for the Chatwin parameter for RCA.DAT sampling station data file.

9. ASSOCIATED COMPUTER PROGRAMS

To facilitate the efficient use of QTRACER, three additional programs have been developed and included with this package. The first, NDATA, allows the user to run an efficient interpolation program to fill missing data in either the time-concentration or the time-discharge data files. The second program, AUTOTIME, converts time-concentration data files using military time into sequential decimal time as required by QTRACER. The third program, DATFILE, provides a straightforward interface for the creation of a sample station datafile.

The results of these three programs are easily appended or copied to a *.DAT file (see Section 6.6.24. and the end of Figure 15). By judicious use of these programs QTRACER can be made more efficient because the data can be so quickly and easily placed in required form.

9.1. NDATA COMPUTER PROGRAM

Typically, discharge is not measured as frequently or at the same time as tracer concentration. Hence, the time concentration data file might appear as (no specific data file example):

```
0.0 0.00 4.10
1.0 2.05
5.0 4.50 3.96
10.0 4.10
15.0 4.33
20.0 0.03 3.80
```

Clearly the data file cannot be processed, because values for discharge and corresponding values for concentration must also be recorded in the file (unless a constant discharge was listed above). To resolve this problem a very good data interpolation algorithm has been programmed (same one used in QTRACER) as NDATA.EXE. To use this program just type NDATA at the DOS prompt and follow the instructions. However, it will ONLY work on a straight time-concentration file or time-discharge file without any other headers. Therefore the algorithm must be used on the original data set(s) and the results copied to the bottom on the final data file to be processed.

When using NDATA only X/Y data can be read in by the program as a data file. So if you were missing some discharge values, create a set of X/Y values in which time values correspond to X and discharge values correspond with Y. Do not use the concentration

values. The program can then be used to fill in missing discharge values. When typing in the data OMIT all time values for which a corresponding discharge or concentration value is missing. Using the example above, if concentration value corresponds to time=15.0 the user would exclude the entire line from the data set to be processed. Obviously, the greater the number of missing data pairs, the greater the interpolation errors.

Note that NDATA is to be used to fill data gaps in both concentration data and discharge, but only where corresponding values are missing. It is better to allow QTRACER to perform data interpolation on a complete data file.

9.1.1. NDATA Source

The FORTRAN source code is included on the NDATA disk. Modification of the NDATA main file can be relatively easily accomplished if desired, but is not recommended. The user should not attempt to modify the included subroutines.

9.2. AUTOTIME COMPUTER PROGRAM

Tracer-breakthrough curve data is often recorded in military time as opposed to sequentially from 0 to infinity. AUTOTIME will convert data recorded in military time into sequentially listed time in terms of decimal seconds, decimal minutes, decimal hours, or decimal days depending on the user's preference.

The user must first create a time-concentration file such as is shown in Figure 40.

Type `AUTOTIME` and then follow the instructions to create a new file of time-concentration data that can then be copied to the bottom of a *.DAT file to be read by QTRACER. Note that the concentration and discharge values are not altered by AUTOTIME. Also note that a variable discharge recorded by the user is allowed in a third column that is read by AUTOTIME. The third column is not necessary, however.

Running AUTOTIME on the data listed in Figure 40 for conversion to decimal hours will result the file listed in Figure 41. It will be remembered that QTRACER allows for free-format data entry so a nicely lined up data column is unnecessary. All that is necessary is that the two data columns be separated by at least one blank space or one comma.

9.2.1. AUTOTIME Source

The FORTRAN source code is included on the AUTOTIME disk. Modification of the AUTOTIME main file can be relatively easily accomplished if desired, but is not recommended.

```
10 15 0.010 3.23E-2
21 45 0.010 3.23E-2
22 15 0.060 3.23E-2
22 45 0.500 3.23E-2
23 15 1.320 3.23E-2
23 45 2.050 3.23E-2
0 15 3.900 3.23E-2
0 45 4.200 3.23E-2
1 15 4.200 3.23E-2
1 45 3.400 3.23E-2
2 15 3.050 3.23E-2
2 45 2.450 3.23E-2
3 15 2.000 3.23E-2
3 45 1.500 3.23E-2
4 15 1.200 3.23E-2
4 45 0.950 3.23E-2
5 15 0.800 3.23E-2
5 45 0.600 3.23E-2
6 15 0.550 3.23E-2
6 45 0.500 3.23E-2
7 15 0.420 3.23E-2
7 45 0.370 3.23E-2
8 15 0.350 3.23E-2
8 45 0.300 3.23E-2
13 45 0.200 3.23E-2
22 45 0.010 3.23E-2
```

Figure 40. Example of a sample time-concentration file using military time for conversion (Mull et al.., 1988).

```
0.000000E+00 1.000000E-02 3.230000E-02
11.500000 1.000000E-02 3.230000E-02
12.000000 6.000000E-02 3.230000E-02
12.500000 5.000000E-01 3.230000E-02
13.000000 1.320000 3.230000E-02
13.500000 2.050000 3.230000E-02
14.000000 3.900000 3.230000E-02
14.500000 4.200000 3.230000E-02
15.000000 4.200000 3.230000E-02
15.500000 3.400000 3.230000E-02
16.000000 3.050000 3.230000E-02
16.500000 2.450000 3.230000E-02
17.000000 2.000000 3.230000E-02
17.500000 1.500000 3.230000E-02
18.000000 1.200000 3.230000E-02
18.500000 9.500000E-01 3.230000E-02
19.000000 8.000000E-01 3.230000E-02
19.500000 6.000000E-01 3.230000E-02
20.000000 5.500000E-01 3.230000E-02
20.500000 5.000000E-01 3.230000E-02
21.000000 4.200000E-01 3.230000E-02
21.500000 3.700000E-01 3.230000E-02
22.000000 3.500000E-01 3.230000E-02
22.500000 3.000000E-01 3.230000E-02
27.500000 2.000000E-01 3.230000E-02
36.500000 1.000000E-02 3.230000E-02
```

Figure 41. Example of a converted sample time-concentration file created by AUTOTIME (Mull et al., 1988).

9.3. DATFILE COMPUTER PROGRAM

The easiest method of creating a sample station data file (Figure 15) may be accomplished by using a PC editor to edit an existing sample station data file and saving the altered file using a new *filename*. However, if desired, the user may use DATFILE to create a sample station data file.

To use DATFILE the user need only type `DATFILE` and respond to each requestor in turn. DATFILE incorporates AUTOTIME so that data listed in military time may be directly converted to sequential decimal time. It also allows the user to enter an existing file of time-concentration data (using military time or sequential decimal time) to be incorporated in the sample station data file to be created.

It will be noted that a sample station data file created using DATFILE will not appear exactly in the form of Figure 15 because of some formatting differences. This is not a problem because QTRACER uses free format for input.

9.3.1. DATFILE Source

The FORTRAN source code is included on the DATFILE disk. Modification of the DATFILE main file can be relatively easily accomplished if desired, but is not recommended.

10. CONCLUSIONS

Tracer-breakthrough curves developed from quantitative ground-water tracing studies in karst and fractured-rock aquifers can be evaluated given the present high level of accuracy of analytical fluorescence chemistry and efficiency of numerical algorithms available. Ground-water flow directions, velocities, and related hydraulic processes such as dispersion, divergence, convergence, dilution, and storage can be properly established from tracer studies and can be used to devise better structural models of the karst aquifer. Because of the lack of physical access to caves at many karst sites, these structural models can be valuable for predicting ground-water flow and contaminant transport in the aquifer.

From a human health perspective, quantitative ground-water tracing studies can assist in demonstrating real connections between tracer injection sites and downgradient receptors. Residence times and tracer velocities can provide ground-water managers with potential time-of-travel estimates likely to occur for nonreactive pollutant spills in the vicinity of tracer injection sites. Pollutant mass dispersion, dilution, and related processes can also be estimated by such studies. Until such time that conduit accessibility becomes a reality, ground-water tracing studies provide the best alternative to acquiring hydraulic data for karst and fractured-rock aquifers.

A robust, efficient, easy-to-use computer program, QTRACER, and two related computer programs, NDATA and AUTOTIME, facilitate the analysis of tracer-breakthrough curves. All three programs are well documented. It is expected that in the future, quantitative tracing of contaminated sites will become more and more important for parameter estimation. QTRACER will enhance the necessary analyses and lead to improved site evaluations.

NOTATION

A	cross-sectional area (L^2)
A_I	accuracy index (dimensionless)
A_p	constant of proportionality for amount of diffusing material (M $T^{1/2}$ L^{-3})
A_s	karst conduit surface (L^2)
C	tracer concentration (M L^{-3})
C_0	initial tracer concentration (M L^{-3})
C_f	final tracer concentration (M L^{-3})
$\bar{C}_i$	average concentration of tracer input over time interval (M L^{-3})
C_p	peak tracer concentration (M L^{-3})
C_{pL}	steady-state (plateau) tracer concentration at a resurgence for repeated instantaneous injections (M L^{-3})
$C(x_s, t)$	mass of recovered tracer over distance(s), x_s and time(s), t [M L^{-3}];
d	pipe diameter (L)
D	steady-state tracer dilution for multiple injections (dimensionless)
D_C	karst conduit diameter (L)
D_H	karst conduit hydraulic depth (L)
D_L	longitudinal dispersion coefficient (L^2 T^{-1})
D_m	molecular diffusion coefficient (L^2 T^{-1})
f_f	friction factor (dimensionless)
g	gravitational acceleration (L T^{-2})
h_L	hydraulic head loss (L)
k_f	mass transfer coefficient (L T^{-1})
K	equivalent hydraulic conductivity for laminar flow (L T^{-1})
K_a	karst conduit sorption coefficient (L)
m	karst conduit roughness correction factor (dimensionless)
M_{in}	mass of tracer injected (M)
M_m	mass of multiple tracer injections (M)
M_O	mass of tracer recovered (M)
M_T	total tracer mass recovered from all sampling stations (M)
n_e	effective fracture porosity (dimensionless)
N_F	Froude number (dimensionless)
N_R	Reynolds number (dimensionless)

N_{sc} Schmidt number (dimensionless)

N_{sh} Sherwood number number (dimensionless)

Pe Peclet number (dimensionless)

Q ground-water discharge ($L^3\ T^{-1}$)

$\bar{Q}$ mean ground-water discharge ($L^3\ T^{-1}$)

r karst conduit radius (L)

t time of sample collection (T)

t_p time to peak concentration (T)

$\bar{t}$ mean tracer residence time (T)

Δt time interval between multiple tracer injections (T) and

$\bar{\upsilon}$ mean tracer velocity ($L\ T^{-1}$)

υ_p peak tracer velocity ($L\ T^{-1}$)

υ_s shear tracer velocity ($L\ T^{-1}$)

x_s radial distance to sampling station (L)

V volume of individual karst conduits or fractures (L^3)

V_T total volume space occupied by open space used for tracer migration L^3)

w fracture width (L)

x straight-line tracer migration distance (L)

x_s sinuous tracer migration distance $= 1.5x$ (L)

Greek

δ laminar flow sublayer (L)

δ_m molecular diffusion layer thickness (L)

ε relief of karst conduit wall surface irregularities (L)

μ dynamic viscosity ($M\ L^{-1}T^{-1}$)

π pi (dimensionless)

ρ fluid density ($M\ L^{-3}$)

σ_t standard deviation for mean residence time (T)

σ_υ standard deviation for mean flow velocity ($L\ T^{-1}$)

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