# The QTRACER2 Program for Tracer-Breakthrough Curve Analysis for Tracer Tests in Karstic Aquifers and Other Hydrologic Systems

(Supersedes EPA/600/R-98/156a and 156b, 2/'99)

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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 (BTCs) generated from tracing studies conducted in hydrologic systems. 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 contamination problems in hydrological systems. 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.

QTRACER2 is an update of the original QTRACER package (Field, 1999) which was intentionally limited to fractured-rock and karstic aquifers. QTRACER2 addresses hydrological-tracer tests conducted in all types of hydrological systems. These hydrological systems include surface-water streams, granular aquifers, fractured-rock aquifers, and subsurface-flow channels (*e.g.*, mine tunnels, solution conduits, *etc.*). By necessity, some hydrological systems are more amenable to certain types of analyses than are other hydrological systems for the given information. For example, granular aquifers are not amenable to head-loss estimation without an estimate for hydraulic conductivity. Much of the original discussion material contained in QTRACER has been retained here because of the necessity of emphasizing the value of quantitative tracer tests in general and in karst aquifers in particular.

Another improvement included in QTRACER2 is the ability to provide correct moment analyses for pulse and continuous releases. The original QTRACER package was intentionally limited to impulse releases because it was believed that most if not all tracer tests conducted in fractured-rock and karstic aquifers consist of impulse releases. However, because short-pulse releases are commonly employed in other systems and long-pulse releases are sometimes employed, it was deemed appropriate to include analyses for these types of releases. Continuous releases are much less commonly applied, but the analyses are the same as for long-pulse releases.

The changes applied in QTRACER2 required modifications to the original input files read by QTRACER. These changes are documented in this report. Also, to bring QTRACER2 up-to-date with current PC operating systems (*e.g.*, Windows®) it was

necessary to reformulate much of the computer graphics which resulted in a loss in some functionality and an increase in others.

Lastly, minor bugs discovered in the original QTRACER package after publication have been corrected in QTRACER2. While no guarantee that QTRACER2 is bug free can be provided, every effort has been made to identify and eliminate any bugs that may exist.

# AUTHOR AND REVIEWERS

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 testing is generally regarded as the most reliable and efficient method of gathering surface and subsurface hydraulic information. This is especially true for karstic 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 karstic sites in the United States, although it is widely recognized that they provide a wealth of hydraulic and geometric data and are commonly employed in nonkarstic hydrological systems. Quantitative tracer tests are regarded as more difficult and time-consuming than qualitative tracing tests, which is a fallacy that needs to be overcome. The benefits of quantitative tracing far outweigh any additional expenses incurred for all hydrologic systems.

An efficient, reliable, and easy-to-use computer program, QTRACER2, designed to run on PCs running any version of Microsoft Windows®, has been developed to facilitate tracer-breakthrough curve (BTC) analysis. It solves the necessary equations from user-generated data input files using robust integration routines and relies on established hydraulic models. Additional features include dynamic memory allocation, the 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.

Four other programs are included to facilitate the use of QTRACER2. The first, NDATA, allows users to interpolate either their time-concentration or time-discharge data files to fill in data gaps. The second program, AUTOTIME, allows users to convert time-concentration data files recorded using military time (a 24-hour clock) into sequential decimal time as required by QTRACER2. Files created by these two programs may be combined and appended to the bottom of a sampling station data file that can then be read by QTRACER2.

The easiest method for creating a new data-input file for use in QTRACER2 is to modify an existing data-input file using a standard text editor (e.g., Notepad) and save the revised file with a new name. However, if desired the user may access the third additional program, DATFILE, to create or modify a data-input file by answering a series of querries posed by the program.

Lastly, the fourth program was designed to address the problem of non-matching time-concentration and time-discharge data. The program, COMBINE, combines two disparate time-data sets into one time-concentration-discharge data set for use by Qtracer2.

# 1. INTRODUCTION

Quantitative tracing studies in hydrological systems are studies designed to provide detailed information regarding flow dynamics. Such flow dynamics information generally cannot be obtained from qualitative ground-water tracing studies (commonly employed in karstic solution conduits), 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

QTRACER2 was written to be as comprehensive as possible. However, as with any report of this nature, it is necessarily limited in several areas. For example, one limitation that will be obvious to modelers is the nonincorporation of solute-transport theory in the form of transport equations. QTRACER2 was intended for tracer test analysis using the method of moments the results of which can then be used in any number of solute-transport equations in either the direct or inverse modes. Other more basic limitations are also evident in this report.

### 1.1.1. Limitations Related to Type of Tracer

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 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.

### 1.1.2. Types of Applicable Hydrological Systems

While most of this report focuses on tracing karst aquifers to define environmental problems, other hydrological systems are also considered. Karstic aquifers are commonly considered to be the aquifers most in need of tracing studies. Many professional hydrologists are beginning to realize, however, that fractured-rock aquifers are just as much in need of tracing studies

as are karstic aquifers, but in general, tracing fractured-rock aquifers still receives minimal acceptance beyond basic research projects. Assessments of surface-water streams, granular aquifers, and other hydrological systems (*e.g.*, glacial-outwash streams, mine shafts, *etc.*) also benefit from tracing studies.

### 1.1.3. Quantitative Versus Qualitative Tracer Tests

Many aspects of quantitative tracing studies are no different than those of qualitative tracing studies. The main difference is the level of information desired. The studies by Gaspar (1987a,b), Mull *et al.* (1988), and Käß(1998) contain discussions regarding tracer tests. Readers must decide for themselves if a qualitative tracing test is sufficient or if a the more detailed quantitative tracing test will better meet their needs. It is the opinion of the author, and many other tracing professionals, that qualitative tracer tests (and/or the ridiculous term, semi-quantitative tracer tests) are no longer acceptable and should never be considered in lieu of quantitative tracer tests.

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, although tracer-injection methodology is also important.

### 1.1.4. Limitations Based on Test Design

Finally, it is important to note that QTRACER2 (and its predecessor, QTRACER [Field, 1999]) is intended for evaluating the results of tracer tests already conducted. QTRACER2 is wholly dependent on the quality of the data developed during the tracer test, which requires good tracer-test design and implementation prior to analysis. This report does not attempt to address either the design or implementation aspects of a tracer test. For a comprehensive discussion and applicable methodology of tracer-test design, the reader is referred to Field (2002a,b,c,d). For discussions regarding tracer-test implementation, the reader should examine several of the references listed at the end of this report.

### 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 karstic and fractured-rock aquifers, ground-water monitoring can be extremely difficult. The main purpose of this document is to illustrate the advantages of conducting quantitative tracing tests and to introduce the computer program, QTRACER2 for tracer-breakthrough curve (BTC) analysis.

QTRACER2 is an efficient, reliable, and easy-to-use computer program designed to run on PCs running any version of Microsoft Windows®. It was developed to facilitate BTC analysis. QTRACER2 solves the necessary equations from user-generated data input files using robust integration routines and by relying on established hydraulic models. Additional features include dynamic 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 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 vadose 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 the 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 (especially in karstic 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).

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

### 1.2.3.  Quantitative Tracer Tests for Solute-Transport Parameter Estimation

In some instances, it may be desirable to model the hydrologic 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 that are 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 and Pinsky (2000) 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 the case. In other instances, additional details of the aquifer under investigation need to be established.

It has been suggested that quantitative tracing studies are too expensive because (1) required sampling at a frequency sufficient to yield reliable results, and (2) the many possible

places the tracer might go, both situations requiring frequent sample collection at tens or even hundreds of locations. Neither of these objections are valid.

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 requirements, but automatic water samplers do not draw very much power and can be run on battery power for long periods.



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

Quantitative tracing studies have proved that a generalized estimate for ground-water flow direction(s), 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. 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. Quantitative tracing studies can also provide significantly better insights into the functioning of the hydrological system than qualitative tracing tracing studies. Reliable estimates for tracer mass recovery, mean residence times, mean ground-water flow velocities, longitudinal dispersion, and maximum volume contact by the tracer allow for useful evaluations of the hydraulic processes of dispersion, divergence, convergence, dilution, and 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. Simple measurement errors may occur as a result of tracer-specific effects, inappropriate sampling, and/or inappropriate analysis (Smart, 1988a). Smart and Laidlaw (1977), as well as 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, their dye names, and 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 |

Appropriate sampling efforts and frequencies for both tracer dye and discharge exert considerable influence on the accuracy of quantitative dye-tracing studies. Analytical

**RHODAMINES**

**XANTHENES**



Sodium Fluorescein

Rhodamine B

Rhodamine WT

Eosin

Sulpho Rhodamine G

Sulpho Rhodamine B

**STILBENES**

**FUNCTIONALIZED POLYCYCLIC AROMATIC HYDROCARBONS**

Tinopal CBS-X

Tinopal 5BM GX

Lissamine Flavine FF

Pyranine

Diphenyl Brilliant Flavine 7GFF

Phorwite BBH Pure

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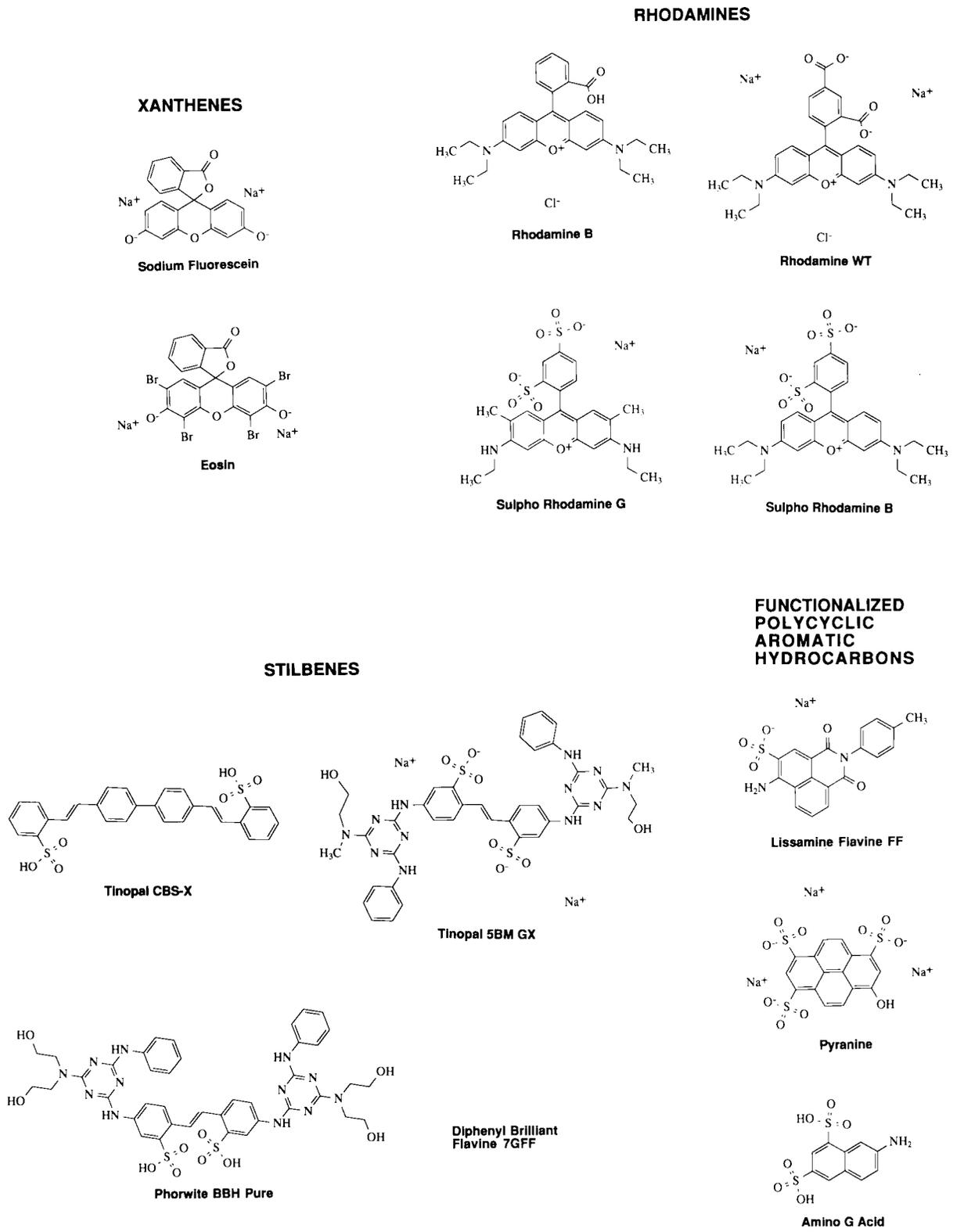
Figure 3. Chemical structures for selected fluorescent dyes used for water tracing.

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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 $\lambda$ (nm) | Maximum Emission[1] $\lambda$ (nm) | Fluorescence Intensity (%) | Detection Limit[2] ($\mu$g 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.  $p$H $\geq 10$
4.  $p$H $\leq 4.5$
Source: Behrens, 1986., Worthington, *pers. comm.*

Tracer tests in karstic and fractured-rock aquifers may be additionally affected by unknown subsurface pathways. Different types of solution-conduit and fracture-flow networks will have a significant effect on tracer mass recovery, but this 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.
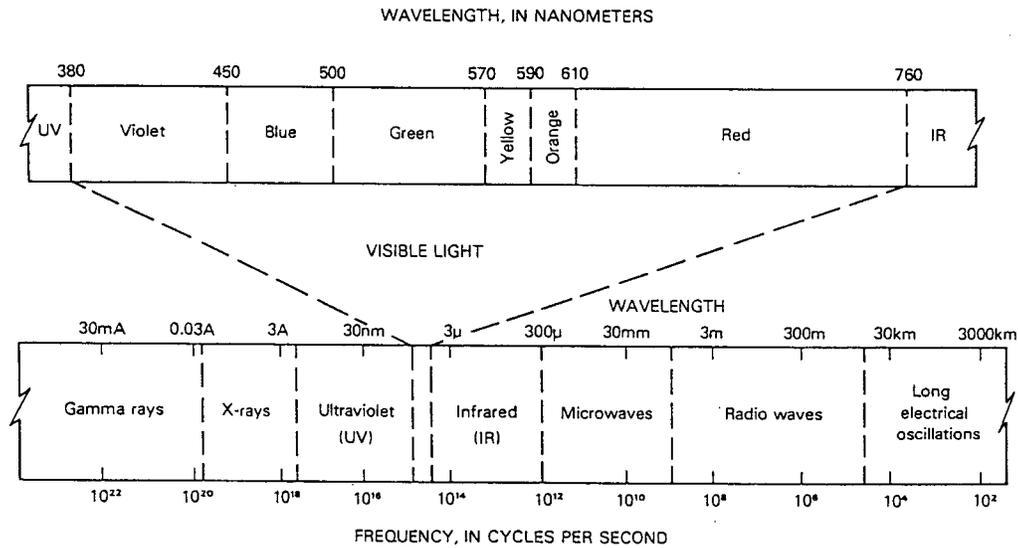
Figure 4. Electromagnetic spectrum with enlargement of visible spectrum for tracer dyes. Modified from Wilson *et al.* (1986, p. 3).

## 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 hydrologic systems 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). For example, sodium fluorescein (Acid Yellow 73) naturally photodecays, which is problematic for surface-water tracer tests.

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

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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 1.19 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$^3$], $\rho$ 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 $3.785 \times 10^{-3}$ is a conversion factor.

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

$$7.570 \times 10^3 \text{ cm}^3 \times 1.19 \text{ g cm}^{-3} \times 1.75 \times 10^{-1} = 1.61 \times 10^3 \text{ g}$$
$$= 1.61 \text{ kg}$$

Subsequent quantification calculations would then use 1.61 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, the commonly used tracer dye, 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 be achieved only 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 a fairly involved process.

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 solution-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.

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 karstic aquifer. Boreholes and wells, in general, are rarely connected to the subsurface flow system.

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

### 2.2.1. Methods of Injection

Tracer injection can be achieved using 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

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.

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 recorded. The contents of the carboy are then easily released into the injection point (Figure 8).

Many of the commonly used fluorescent dyes that were previously available in powder form are now available in liquid form. The liquid form of the powder dyes exhibit greatly reduced concentrations when compared with the powder form (Table 3), but the

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.

concentration is insignificant when mass is used to determine the appropriate tracer mass. Given the availability of liquid dyes there appears to be no useful or valid reason for using the powder form.

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 lubricate the system and to flush out any debris. 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. Experience has

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 a dark red color when concentrated as shown here, but becomes a bright fluorescent green when diluted.

Table 3. Percent pure dye content for selected fluorescent dyes.

| Colour Index Generic Name | Powder Dye (%) | Liquid Dye (%) | Specific Gravity (g cm$^{-3}$) |
|---|---|---|---|
| Acid Blue 9 | 74.0* | 37.0 | — |
| Acid Red 52 | 90-92.0 | 18.0 | 1.175 |
| Acid Red 87 | 86.0 | 26.0 | — |
| Acid Red 388 | 85.0** | 17.0 | 1.160 |
| Acid Yellow 73 | 60.0 | 30.0 | 1.190 |
| Basic Violet 10 | 90.0 | 45.0† | — |
| Fluorescent | | | |
|     Brightener 351 | 60.0 | — | — |
| Solvent Green 7 | 80.0 | — | — |

Values listed are equal to within ±5.0%.
*Acid Blue is also sold with a Food, Drug and Cosmetic (FD&C) purity equal to 92.0%.
**Acid Red 388 is not commercially available in powder form.
†Basic Violet 10 as a liquid is mixed with glacial acetic acid.
Note: The values listed are specific to one manufacturer; crude dye stocks can and will vary significantly with manufacturer.

shown that a slow flow (*e.g.*, ≤ 50 gpm) is more effective than a rapid flow.

## 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 semi-quantitative. Sampling must also be of sufficient frequency 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 go unobserved.

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 to minimize losses. Automatic samplers can be programmed to collect a water sample at appropriate sampling frequencies so that even late-night 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 × 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 be collected if fluorescent dyes are used as tracers. It is believed that activated charcoal will ensure dye recovery because the supposed 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 (Smart and Karunaratne, 2001; Smart and Simpson, 2001).

## 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 before 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, resulting in added costs (excessive number

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of samples collected) or inadequate tracer mass recovery (too few samples collected too infrequently). Preliminary simple ground-water tracing studies can be useful for more difficult and complicated tracing studies. However, as previously discussed (Section 1.3. on page 5), 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 FLOW SYSTEM

Complete lateral and vertical mixing of the tracer 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 does not always ensure that adequate lateral mixing will occur in solution 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 the spring and the BTC plotted for each sampling point in the cross-section. Complete lateral mixing is determined to have occurred when the areas under the BTCs, 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 TIME TO REACH FLOW SYSTEM

For some tracer injections, accurate time of travel, velocity, and dispersion estimates require that the time needed for the tracer to reach the flow system (*e.g.*, infiltration time) be taken into account for a more accurate estimate. Tracer flow velocity is adjusted for time to reach and/or exit the flow system by subtracting $t_{inf}$ from the total real time of travel values $t_i$ and integrating. However, this will lead to negative times of travel, so it is easier to subtract $t_{inf}$ from the mean time of travel $\bar{t}$ to obtain the true tracer velocity (Dole, 1906, p. 78)

$$\bar{v} = \frac{x}{\bar{t} - t_{inf}} \tag{2}$$
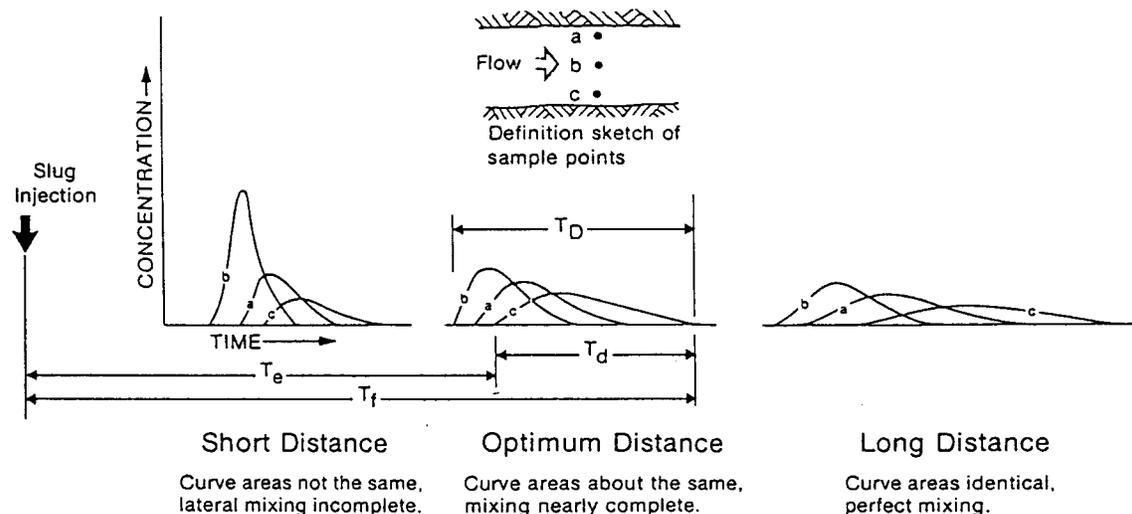
Figure 9. Typical response curves observed laterally and at different distances downstream from a slug injection of a tracer in the center of a stream where the symbols are defined in the Notations section (page 172) (Kilpatrick and Cobb, 1985, p. 3).

The difference between the true velocity and the perceived velocity is then (Dole, 1906, p. 78)

$$\bar{v} = \frac{x\,t_{inf}}{(\bar{t} - t_{inf})\bar{t}} \tag{3}$$

with a consequent correction for dispersion. While this adjustment is usually not necessary for surface-water tracer tests and many tracer injections into disappearing streams and sinkholes, it may be absolutely essential for accurate analyses for deep aquifers, or slow infiltration through the beds of sinking streams.

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

Prior to any tracing efforts, background water samples $C_{b_i}$ need to be collected and analyzed for the tracer of interest. If the values obtained are low enough (*e.g.*, few $\mu$g L$^{-1}$),

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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 $\overline{C_b}$ because it is not possible to subtract a suite of background concentrations from the measured concentrations. This final average background concentration is subtracted from every sample of recovered tracer from subsequent tracing efforts

$$C_{i_f} = C_{i_i} - \overline{C_b} \tag{4}$$

where

$$\overline{C_b} = \frac{1}{n} \sum_1^n C_{b_i} \tag{5}$$

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.

## 2.9.  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 non-pumping 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.

## 2.10. 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 tracer 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.

### 2.10.1. 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.

### 2.10.2. 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 conclusion of a lack of hydraulic connectivity (*i.e.*, if the dye goes elsewhere, such results indicate there is no flow to the sites being monitored).
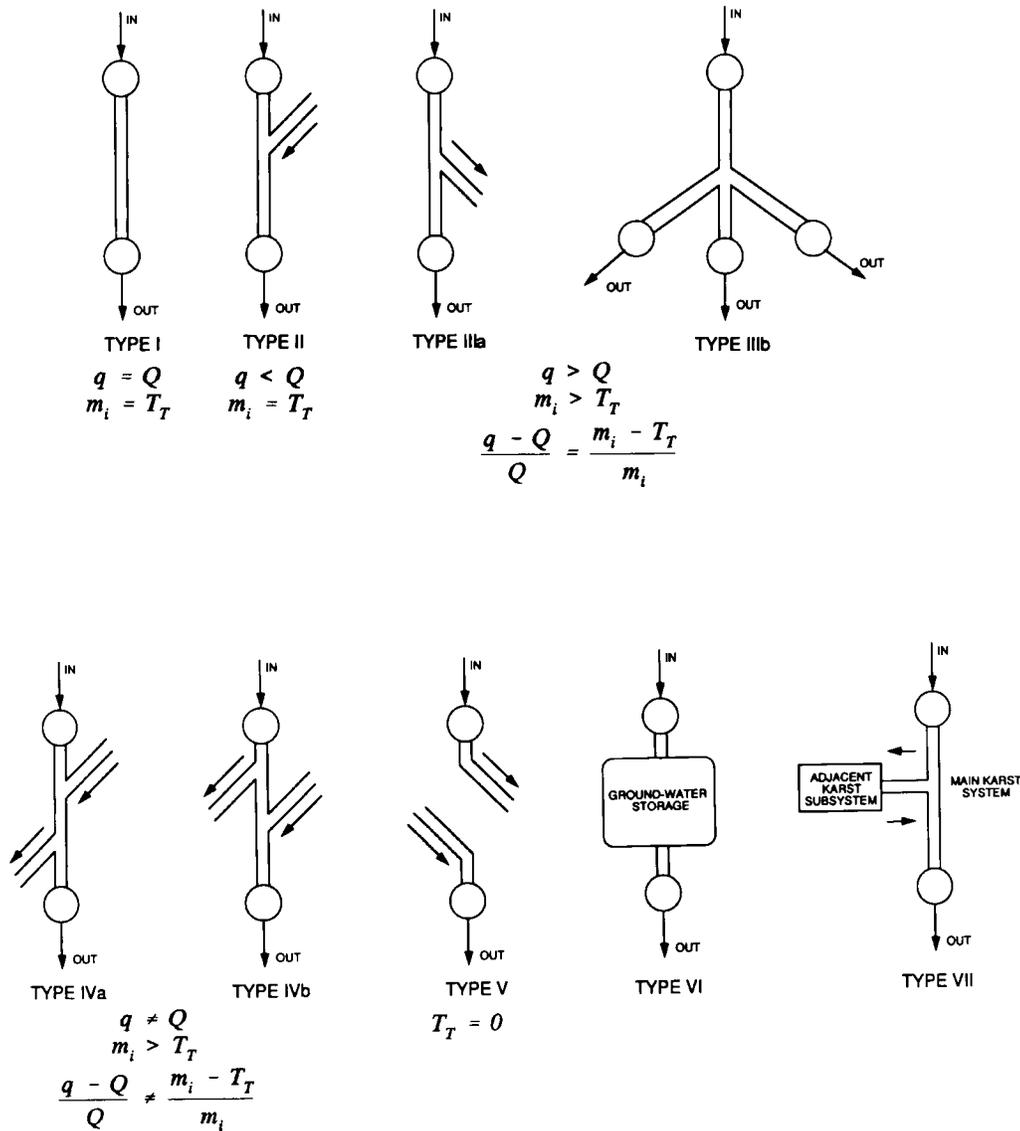
Figure 10. Seven simple karst network types that describe tracer migration in karst conduits. Any of these networks may significantly influence tracer tests between the point of inflow (IN) and the point of outflow (OUT) in a karst system. Discharge into the conduit is $q$, discharge out of the conduit 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).

### 2.10.3. 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 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.

### 2.11. 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 BTCs, 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 hydrological systems depends upon:

- Character of the tracer;

- Prevailing flow conditions;

- Structure of the aquifer (Smart, 1988a);

Discussion of these conditions, as related to BTCs, has already been addressed and 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; and

- 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 BTC (Smart, 1988a). These problems lead to 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 be answered by only making best professional interpretations of the BTC.
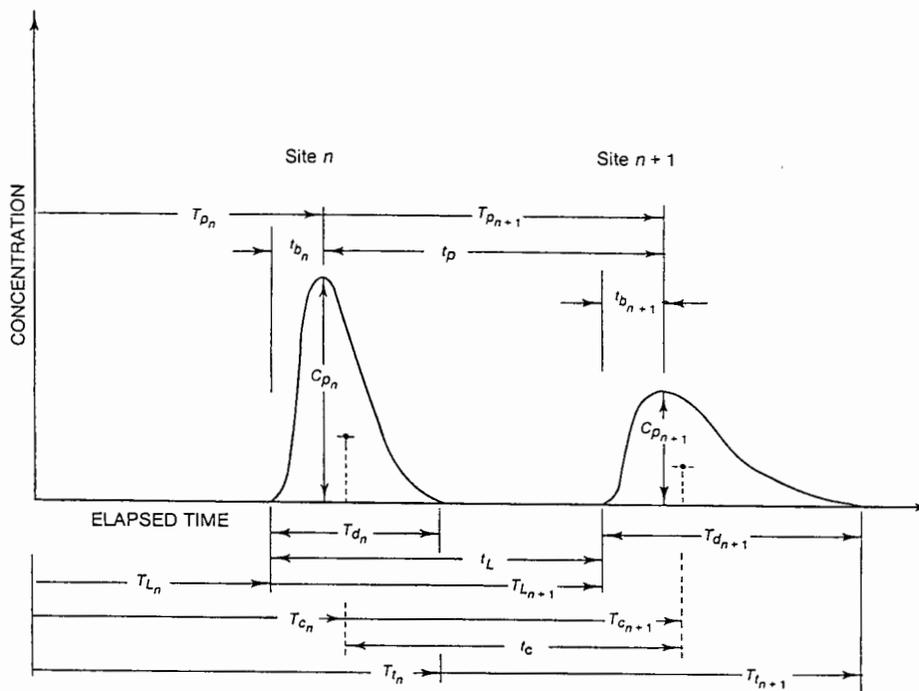
Figure 11. Definition sketch of BTCs along a selected tracer streamline from an instantaneous tracer injection (Kilpatrick and Wilson, 1989, p. 3).

Others may be answered by careful numerical analysis of the BTC. 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 may be 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. The second moment is used to estimate the longitudinal dispersion. However, as will be shown, the second moment may not provide reliable estimates for dispersion (Field and Pinsky, 2000).

   Analysis by the method of moments is nothing more than determining the area under the BTC generated by plotting time versus measured tracer concentrations (Figure 11).

   The following discussion is taken from Kilpatrick and Wilson (1989, p. 3 and 4).

   The BTCs along a streamline shown in Figure 11 may be described in terms of elapsed

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time after a slug injection. Characteristics pertinent to the BTC analysis are:

- $T_L$, elapsed time to the arrival of the leading edge of the BTC *at a sampling point*;

- $T_p$, elapsed time to the peak concentration $C_p$ of the BTC *at a point*;

- $T_c$, elapsed time to the centroid of the BTC *at a point*; and

- $T_t$, 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 BTCs defined upstream and downstream *on the same streamline* given by

$$t_c = T_{c_{n+1}} - T_{c_n} \tag{6}$$

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

$$t_L = T_{L_{n+1}} - T_{L_n} \tag{7}$$

$$t_p = T_{P_{n+1}} - T_{p_n} \tag{8}$$

and

$$t_t = T_{t_{n+1}} - T_{t_n} \tag{9}$$

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

$$T_d = T_{t_n} - T_{L_n} \tag{10}$$

As shown in Figure 11, a typical tracer cloud may travel faster in the center of the stream than along the flow channel walls, where it may also be elongated. Complete definition of the BTC may involve measurement at more than one point or streamline at several sections (if possible). Usually, in hydrologic systems other than surface streams, 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, if possible, 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 flow channel 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 (6)–(10) because it is rare for ground-water tracing studies to provide an opportunity for sampling at multiple locations along a streamline. Direct access to a cave during a tracer test is one exception.

### 3.1.1. Total Tracer Recovery

Estimation of tracer recovery for individual sampling stations is given by Equation (11) (modified from Gaspar, 1987b, p. 62)

$$M_O = \int_0^\infty C(t)\, Q(t)\, dt \tag{11}$$

and total tracer recovery from all downgradient receptors may be estimated from Equation (12) (Gaspar, 1987b, p. 63)

$$M_T = \sum_{i=1}^n M_{O_i} \tag{12}$$

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 mass 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 (11) 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 a percent of mass recovered, but this affords little insight. An accuracy index given by Sukhodolov *et al.* (1997)

$$A_I = \frac{M_{in} - M_T}{M_{in}} \tag{13}$$

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,

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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 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 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 in the BTC, but the more flow conforms to Fick's law, the less obvious the difference between the centroid and the peak concentration.

Mean tracer residence time for impulse and short-pulse releases $(t_2 < \bar{t})$ is estimated from Equation (14) (modified from Gaspar, 1987a, p. 93)

$$\bar{t} = \frac{\int_0^\infty t \, C(t) \, Q(t) \, dt}{\int_0^\infty C(t) \, Q(t) \, dt} \tag{14}$$

and for long-pulse and continuous releases $(t_2 \geq \bar{t})$ from (Sardin *et al.*, 1991)

$$\bar{t} = \int_0^\infty [1 - F(t)] \, dt \tag{15}$$

where

$$F(t) = \frac{C(t)}{C_p} \tag{16}$$

Travel-time variance for impulse and short-pulse releases $(t_2 < \bar{t})$ is estimated from

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Equation (17) (modified from Mull *et al.*, 1988, p. 58)

$$\sigma_t^2 = \frac{\int_0^\infty (t - \bar{t})^2\, C(t)\, Q(t)\, dt}{\int_0^\infty C(t)\, Q(t)\, dt} \tag{17}$$

and for long-pulse and continuous releases $(t_2 \geq \bar{t}\,)$ from (Sardin *et al.*, 1991)

$$\sigma_t^2 = 2 \int_0^\infty [1 - F(t)] t\, dt - \bar{t}^2 \tag{18}$$

It will be noted that for Equations (17) and (18) to be appropriate for long-pulse releases, the time-concentration data file must be truncated so that the descending time-concentration data is ignored in the calculations.

Equations (14) to (18) 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 also be confused with Equation (14). A simplified example calculation is performed later in this report (see Section 4. on page 48).

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 water managers with an indication of the length of time a contaminant will take to be detected at a downgradient receptor. However, the effects of longitudinal dispersion and inadequate sensitivity of current analytical methods at extremely low concentrations render this situation meaningless.

### 3.3. Residence Time Skewness and Kurtosis

Tracer travel time skewness is a measure of the lateral asymmetry of the BTC and the kurtosis is a measure of the peakness of the BTC. For impulse and short-pulse releases, skewness may be determined from (modified from Mull et al., 1988, p. 58)

$$\gamma_t = \frac{\displaystyle\int_0^\infty (t - \bar{t})^3 \, Q(t) \, C(t) \, dt}{\sigma_t^3 \displaystyle\int_0^\infty Q(t) \, C(t) \, dt} \tag{19}$$

and the kurtosis may be determined from

$$\kappa_t = \frac{\displaystyle\int_0^\infty (t - \bar{t})^4 \, Q(t) \, C(t) \, dt}{\sigma_t^4 \displaystyle\int_0^\infty Q(t) \, C(t) \, dt} \tag{20}$$

For continuous and long-pulse releases, the calculation of skewness is considerably more difficult. In this instance skewness may be obtained from (Ravi Subramaniam, *pers. comm.*)

$$\gamma_t = \frac{\displaystyle\int_0^\infty [3 - F(t)] \, t^2 \, dt - 6\,\bar{t} \displaystyle\int_0^\infty [1 - F(t)] \, t \, dt + 2\,\bar{t}^3}{\left(\sigma_t^2\right)^3} \tag{21}$$

and the kurtosis may be determined from

$$\kappa_t = \int_0^\infty [4\,t - 12\,\bar{t} - F(t)] \, t^2 \, dt + 12\,\bar{t}^2 \int_0^\infty [1 - F(t)] \, t \, dt - 3\,\bar{t}^4 - 3\left(\sigma_t^2\right)^2 \tag{22}$$

A symmetrical curve results in a skewness coefficient equal to zero. Positive number for the skewness indicates that the BTC is weighted to the right, recedes more gently than it rises (Mull *et al.*, 1988, p. 59), and reflects both longitudinal dispersion and dead zone effects. Skewness is used by Qtracer2 only for comparison of dimensionless BTCs generated from multiple tracer tests conducted from the same injection points to the same recovery locations as described by Mull et al. (1988). Kurtosis is also used by Qtracer2 for comparison purposes only for comparison of dimensionless BTCs generated from multiple tracer tests conducted from the same injection points to the same recovery locations. Application of skewness and kurtosis estimates is briefly discussed in Section 6.6.21. on page 86

### 3.3.1. Mean Tracer Velocity

Mean tracer velocity is a measure of the flow rate of the centroid of the tracer mass. For impulse releases, mean tracer velocity is given by Equation (23) (modified from Gaspar,

1987b, p. 66)

$$\bar{v} = \frac{\displaystyle\int_0^\infty \frac{x_s}{t}\, C(t)\, Q(t)\, dt}{\displaystyle\int_0^\infty C(t)\, Q(t)\, dt} \tag{23}$$

with a standard deviation for impulse releases given by Equation (24)

$$\sigma_v = \sqrt{\frac{\displaystyle\int_0^\infty \left(\frac{x_s}{t} - \frac{x_s}{\bar{t}}\right)^2 C(t)\, Q(t)\, dt}{\displaystyle\int_0^\infty C(t)\, Q(t)\, dt}} \tag{24}$$

For short-pulse releases $(t_2 < \bar{t})$, mean tracer velocity is given by Equation (25)

$$\bar{v} = \frac{\displaystyle\int_0^\infty \frac{x_s}{t - t_2/2}\, C(t)\, Q(t)\, dt}{\displaystyle\int_0^\infty C(t)\, Q(t)\, dt} \tag{25}$$

with a standard deviation given by Equation (26)

$$\sigma_v = \sqrt{\frac{\displaystyle\int_0^\infty \left[\left(\frac{x_s}{t - t_2/2} - \frac{x_s}{\bar{t} - t_2/2}\right)\right]^2 C(t)\, Q(t)\, dt}{\displaystyle\int_0^\infty C(t)\, Q(t)\, dt}} \tag{26}$$

For long-pulse and continuous releases $(t_2 \geq \bar{t})$, mean tracer velocity is given by Equation (27)

$$\bar{v} = \frac{x_s}{\displaystyle\int_0^\infty [1 - F(t)]\, dt} \tag{27}$$

The standard deviation for long-pulse and continuous releases $(t_2 \geq \bar{t})$ cannot be solved trivially and is not attempted here.

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 solution conduits is unrealistic and should be corrected for sinuosity (Field and Nash, 1997; Worthington, 1991, pp. 85–91) by

$$x_s = S_d\, x \tag{28}$$

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where $1 \leq S_d \leq 3$. Typically, $S_d$ will be about 1.3 to 1.5 for most solution conduits. For surface-water streams and tubes where the length can and has actually been measured or reasonably approximated; (*e.g.*, some traversable caves and mine tunnels) then $S_d = 1.0$ which should also be the accepted value for porous-media flow (unless a tortuosity value is to be considered).

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 (23) and (27) 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 not reproduced here to avoid confusion. An example of its use is presented later in this report (see Section 4. on page 48).

### 3.3.2. Longitudinal Dispersion

Longitudinal dispersion in surface and subsurface channels is similar to dispersion in closed conduits and open channels. This is because conduit flow ranges from slow and laminar to rapid and turbulent in subsurface channels that may exhibit either closed-conduit flow or open-channel flow characteristics. Longitudinal dispersion works similarly for fractured-rock aquifers. The longitudinal dispersion coefficient is a measure of the rate at which a concentrated tracer mass spreads out along the flow path (Mull *et al.*, 1988, p. 59). It is defined as the temporal rate of change in 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.

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 flow channel will generally appear as shown in Figure 12 and less so for a fracture-rock aquifer. In Figure 12, the

responses to a slug of injected tracer are shown *with distance* downstream from a single, center slug injection along selected imaginary streamlines.
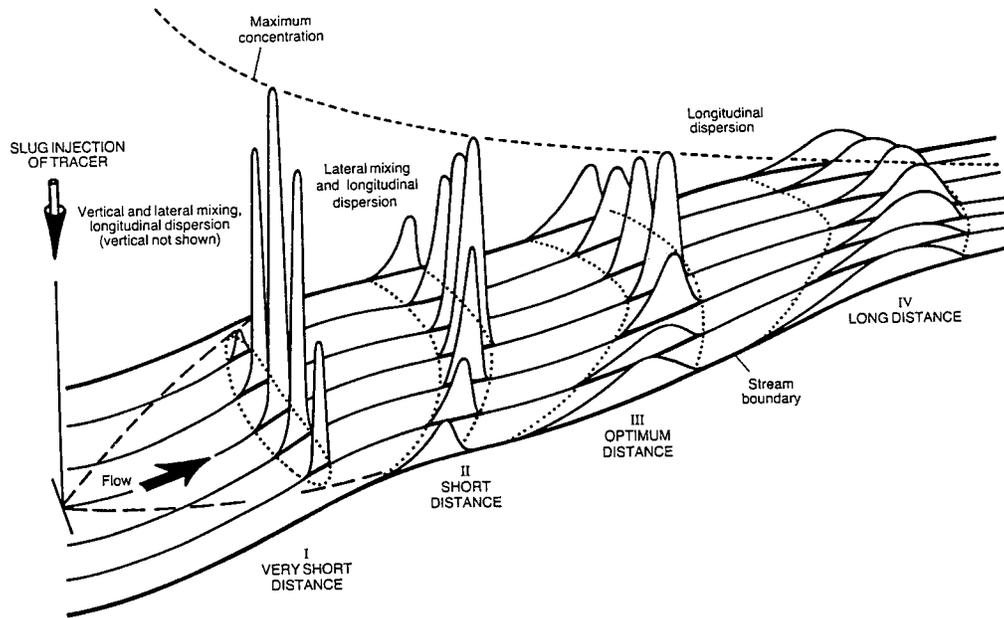


Figure 12. Lateral mixing and longitudinal dispersion patterns and changes in distribution of concentration downstream from a single, center slug injection of tracer (Kilpatrick and Wilson, 1989, p. 2).

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 and its dispersion characteristics will, in effect, be a measure of the movement of an element of fluid in the stream. 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 by the Method of Moments*** Longitudinal dispersion is most commonly estimated using the second moment (Małoszewski and Zuber, 1992), which when properly weighted for concentration, may be estimated for impulse, long-pulse ($t_2 \geq \bar{t}$),

and continuous releases by (Kreft and Zuber, 1978)

$$D_L = \frac{\sigma_t^2 \, v^3}{2x_s} \tag{29}$$

and for short-pulse releases ($t_2 < \bar{t}$) by (Wolff *et al.*, 1979)

$$D_L = \left(\sigma_t^2 - \frac{t_2}{12}\right) \frac{v^3}{2x_s}. \tag{30}$$

It should be recognized here that $D_L$ solved by (30) is based on the assumption of a BTC and does not represent the mean residence time distribution as does (29). In some instances, there will usually not be any major difference in $D_L$ estimation from (29) or (30).

Equations (29) and (30) assume that Fick's law is always applicable; that is, there is no anomalous behavior. In actuality, immobile-flow zones (dead zones) are common, which cause a long tail to the BTC and invalidates Fick's law.

***Longitudinal Dispersion by the Chatwin Method***   Chatwin (1971) developed a method for determining longitudinal dispersion intended to address the problem of non-Fickian behavior. Technically, the Chatwin method is only really valid for impulse releases, but it does provide a reasonable approximation for longitudinal dispersion for pulse and continuous releases (see Section 8.1.1. on page 115). Longitudinal dispersion as developed in Chatwin (1971) is given by Equation (31) as

$$\sqrt{t \ln\left(\frac{A_p}{C\sqrt{t}}\right)} = \frac{x_s}{2\sqrt{D_{x_s}}} - \frac{\bar{v}\,t}{2\sqrt{D_{x_s}}} \tag{31}$$

where the proportionality constant, $A_p$ represents (Davis *et al.*, 2000)

$$A_p = \frac{M}{2\,A\sqrt{\pi\,D_{x_s}}} \tag{32}$$

For symmetrical concentration distributions (Davis *et al.*, 2000),

$$x_s = \bar{v}t \tag{33}$$

$$\overline{C} = C_p = \frac{A_p}{\sqrt{t_p}} \tag{34}$$

which may be rearranged to yield

$$A_p = C_p\sqrt{t_p} \tag{35}$$

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Day (1975) showed that Equation (35) results in relatively insignificant errors for asymmetrical concentration distributions.

Subject to $t_\kappa \leq x_s/\bar{v}$, Equation (31) is reduced to the general least-squares problem by solving

$$\min_x \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 \tag{36}$$

where

$$\mathbf{A} = \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_\kappa \end{pmatrix} \tag{37}$$

$$\mathbf{x} = (x_1, \ x_2)^{\mathrm{T}}, \tag{38}$$

$$\mathbf{b} = (b_1, \ b_2, \ \ldots, \ b_\kappa)^{\mathrm{T}} \tag{39}$$

where T represents the transpose of the vector.

The parameters $b_i$ are equal to the left-hand side of Equation (31)

$$b_i = \sqrt{t_i \ln\left(\frac{A_p}{C\sqrt{t_i}}\right)} \tag{40}$$

and the parameters to be determined $x_i$ are equal to the two factors on the right-hand side of Equation (31)

$$x_1 = \left(\frac{x_s}{2\sqrt{D_{x_s}}}\right) \tag{41}$$

$$x_2 = \left(\frac{\bar{v}}{2\sqrt{D_{x_s}}}\right) \tag{42}$$

where $x_1$ is the y intercept of the straight-line fit to the early-time data and $x_2$ is the slope of the straight-line fit to the early-time data. Either term on the right-hand side allows for solution of the longitudinal dispersion coefficient $D_L$, provided that a plot of the left-hand side of Equation (31) 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).

Equations (29) and (30) tend to overestimate $D_L$, suggesting a greater BTC spread than is likely to occur as a result of solute dispersion. Alternatively, Equation (31) may to underestimate $D_L$ for systems exhibiting Fickian behavior.

In this report, Equation (31) is always used except in those instances where the Chatwin method appears to fail or computer memory storage is exceeded. In that case, Equations (29) and (30) are used as appropriate.

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.

### 3.3.3.   Tracer Dilution

Estimation of tracer dilution is desirable so that effective dilution of pollutant releases may also be estimated. Given the generally nonconservative behavior of most tracers and pollutants in hydrologic systems, 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) of Dobbins (1963).

$$C(x_s, t) = \frac{M_{in}}{A\sqrt{4\pi D_L t}} \exp\left[ \frac{-(x_s - \bar{v}\, t)^2}{4D_L t} \right] \tag{43}$$

Mass $M_{in}$ of the injected tracer is assumed to be small relative to the mass flux rate of the water, so, in theory, the BTC should approach a Gaussian shape. In fact, the BTC is always skewed to the right because of the effects of transverse dispersion (ignored in Equation [43]),

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 BTC (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

$$D = \frac{\overline{C_i}}{C_{pL}} = \frac{M_m}{\Delta t \, Q \, C_{pL}} \tag{44}$$

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

$$C_{pL} = \sum_{j=t_b}^{j=t_b+n\,\Delta t} C_j \tag{45}$$

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 an aquifer is very difficult. Smart (1985) points out that as the tracer is not conserved in the aquifer, 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.

## 3.4.  FLOW-CHANNEL GEOMETRIES

Flow-channel geometries are estimated by evaluating discharge with respect to mean residence time. This is accomplished for either the continuous or the discrete situation. Not all the equations described in this section may be applied to analyses of porous-media systems (*e.g.*, granular aquifers), because of the need to know particle diameter, hydraulic conductivity, and/or other factors.

### 3.4.1. Aquifer Volume

Tracer mass recovery, where discharge was measured during each tracer sampling event, allows for a rough estimate of the maximum volume of flow system traversed by the tracer cloud using of Equation (46) (Atkinson *et al.*, 1973)

$$V = \int_0^{\bar{t}} Q \, dt \tag{46}$$

If a single discharge value is used as a mean discharge, then the volume may be estimated by

$$V = \overline{Q}\,\bar{t} \tag{47}$$

and a total maximum volume estimate based on the sum of each individual transport zone (*e.g.*, solution conduit or fracture) traversed by the tracer cloud may be determined from Equation (48)

$$V_T = \sum_{i=1}^{n} V_i \tag{48}$$

It should be noted that aquifer volume calculations will be only a crude approximation at best. Summing the volumes of individual transport zones to achieve a total maximum volume estimate should not be expected to produce accurate results, but the sum of the individual transport zones do provide some indication of the aquifer volume contacted by tracer. However, Equations (46) and (47) 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 solution conduits and fractures. 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 BTC analyses furnish a means, for assessing the type of karst aquifer under investigation (Atkinson *et al.*, 1973).

### 3.4.2. 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 (46) or (47), the cross-sectional area may be estimated from

$$A = \frac{V}{x_s} \tag{49}$$

where $x_s$ may be a sinuous distance or a straight-line distance. A sinuous distance will result in a smaller $A$ than a straight-line distance would suggest.

### 3.4.3. Flow-Channel Diameter

By assuming a cylindrical flow channel, it is possible to estimate a flow-channel diameter from a BTC. Because the system volume has been estimated, the flow-channel diameter may be obtained by

$$D_C = 2\sqrt{\frac{A}{\pi}} \tag{50}$$

Obviously, $D_C/2$ can be used to estimate the flow-channel radius that is typically used in many modeling endeavors.

### 3.4.4. Flow-Channel Hydraulic Depth

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

$$D_H = \frac{A}{D_C} \tag{51}$$

which is a reasonable approximation.

### 3.4.5. Flow-Channel Surface Area

If the flow channel is assumed to conform to a cylinder, then it is possible to obtain an initial estimate of the conduit surface area. (If it is also a solution conduit, then it needs to conform to Karst Network Types I, II, VI, and VII.) A flow-channel surface area estimate is obtained by

$$A_s = 2\pi r x_s m \tag{52}$$

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 flow channel of interest cannot be directly entered to take physical measurements of roughness.

A reasonable estimate for the roughness factor may be obtained by

$$m = \frac{\varepsilon}{\delta/10^3} \qquad (53)$$

The surface irregularities relief $\varepsilon$, taken as 1.0 m, is considered reasonably representative of typical flow-channel walls. There is some support for this assumption from natural river beds (Chow, 1959, p. 196). The viscous-flow sublayer $\delta$ is divided by $10^3$ in Equation (53) 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 solution conduit he was investigating.

### 3.4.6.   Tracer Sorption Estimation

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

Karst conduit sorption is estimated by

$$K_a = \frac{(C_0 - C_f)V}{C_f A_s} \qquad (54)$$

and for multidischarge systems (*e.g.*, Karst Network Types III and IV)

$$K_a = \frac{(C_0 - C_f)\sum V_i}{C_f \sum A_{s_i}} \qquad (55)$$

If a multidischarge system is of interest, it is essential to note that any results obtained by Equation (54) will be erroneous. Only results obtained by Equation (55) should be considered relevant.

### 3.5.   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 actual

hydrologic 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 solution 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.

### 3.5.1. Péclet Number

The Péclet 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 $\left(-\frac{\bar{v}x_s}{D_{x_s}}\frac{\partial C}{\partial x_s} = -Pe\frac{\partial C}{\partial x_s}\right)$ to the effectiveness of mass transport by either dispersion or diffusion $\left(\frac{\partial^2 C}{\partial x_s^2}\right)$ (Schiesser and Silebi, 1997, p. 372). Péclet 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 nonporous media instances of solute transport in karst conduits, Péclet numbers will be greater than 6.0. Often, the Péclet numbers will be many times greater than 6.0.

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

$$Pe = \frac{\bar{v}\,x_s}{D_{x_s}} \tag{56}$$

It is necessary to note that estimation of the Péclet number by Equation (56) may be too low. Substitution of the peak flow velocity $v_p$ could be considered, but most likely would result in overestimating the Péclet number.

It should also be noted here that even though $x_s$ is listed as representing distance, in reality, for porous-media flow, it probably will not have been corrected for sinuosity.

### 3.5.2. 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. The equations described in this section are not all applicable to analyses of porous-media systems (*e.g.*, granular aquifers) because of the need to know particle diameter.

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***Reynolds Number*** The resistance of flow depends entirely upon the geometry and magnitude of the quantity $\frac{\rho \bar{v} D_C}{\nu}$, where $\rho$ represents fluid density, $d$ conduit diameter, and $\nu$ dynamic viscosity. The Reynolds number $N_R$ 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

$$N_R = \frac{\rho \, \bar{v} D_C}{\nu} \tag{57}$$

Estimation of the Reynolds number by Equation (57) 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 fracture) may be calculated. For laminar flow in a karst conduit, $K$ is obtained by

$$K = \frac{D_C^2 \rho g}{8\mu} \tag{58}$$

and for laminar flow in a fracture, $K$ is obtained by

$$K = \frac{n_e w^2 \rho g}{12\mu} \tag{59}$$

It should be noted that a hydraulic conductivity estimated by either Equation (58) or (59) 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.

For porous-media flow, the Reynolds number uses the hydraulic conductivity in place of the cylinder diameter (de Marsily, 1986, p. 74)

$$N_R = \frac{\bar{v} \, \rho}{\mu} \sqrt{\frac{K \, \mu}{\rho \, g}} \tag{60}$$

although comparisons between Equation (57) and Equation (60) are inappropriate. Using Equation (60) it may be accepted that laminar flow occurs when $1 \leq N_R \leq 10$, transient flow occurs when $10 < N_R \leq 100$, and turbulent flow occurs when $N_R > 100$.

***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

$$N_F = \frac{\bar{v}}{\sqrt{gD_H}} \tag{61}$$

Estimation of the Froude number by Equation (61) 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 subsurface channels may exhibit either open-channel flow, closed-conduit flow, or both flow types depending on stage.

An estimated Froude number for a flow channel exhibiting closed-conduit flow (*e.g.*, karst conduits) is not appropriate. Also, as presented, the calculation for the Froude number assumes that the cross-sectional area of the flow channel, divided by the diameter of the flow channel, is equal to the mean hydraulic depth, which may not always be true.

## 3.6. BOUNDARY-LAYER EFFECTS

While not generally considered in tracing studies, boundary-layer effects can substantially impact the study results. In most instances, flow-channel 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. The equations described in this section are not applied to analyses of porous-media systems (*e.g.*, granular aquifers) because of the need to know particle diameter.

### 3.6.1. Friction Factor Estimation

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

$$f_f = \frac{64}{N_R} \tag{62}$$

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

$$\frac{1}{\sqrt{f_f}} = 2\log\frac{D_C}{\varepsilon} + 1.14 \tag{63}$$

where the relief of surface irregularities $\varepsilon$ is a controlling factor and depends on the nature of the channel through which flow is occurring.

### 3.6.2. Viscous-Flow Sublayer

It is well documented by empirical studies that turbulent flow occurs as a core that is surrounded by a viscous-flow sublayer. The thickness of the viscous-flow sublayer is dependent on the degree of channel-wall roughness. If a typically very rough flow channel is assumed, then the viscous-flow sublayer may be estimated by (White, 1988, p. 163)

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

(64)

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

### 3.6.3. Hydraulic Head Loss

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

$$h_L = \frac{8.0\mu\bar{v}x_s}{\rho g r^2}$$

(65)

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

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

(66)

which emphasizes the influence of friction on head loss.

Hydraulic head loss in porous media is based on a rearrangement of Darcy's law (modified from White, 1988, p. 162)

$$h_L = \frac{\bar{v}\,x_s}{K}$$

(67)

It should be noted here that even though $x_s$ is listed here as representing distance, in reality it probably will not have been corrected for sinuosity.

### 3.6.4. Shear Velocity

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

Estimation of the shear velocity is obtained by

$$v_s = \sqrt{g \frac{A}{D_C} \frac{h_L}{x_s}} \tag{68}$$

It will be noted that flow velocities produced by Equation (68) will always be less than those produced by Equation (23). This makes sense in that the flow channel walls should impart some negative influence (*i.e.*, resistance) on the flow velocity.

## 4. EXAMPLE CALCULATIONS FOR TOTAL TRACER RECOVERY

To determine the total mass recovery of tracer injected into a hydrologic system, 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.

1. **Plot the Concentration** Subtract background tracer concentration. Plot the concentration of tracer recovered (*e.g.*, mg L$^{-1}$) versus 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 sampling location (*e.g.*, spring or well) where discharge is variable over the time of tracer recovery, then plot discharge in appropriate units (*e.g.*, m$^3$ s$^{-1}$) versus time (hours) also. Again, time should be plotted on the x axis. If discharge is constant 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 (11), which must be integrated numerically. This is done using a simple summation algorithm. This is most easily accomplished by setting up a table that facilitates the necessary calculations (Table 4).

Table 4. Table representing tracer recovery data for processing.

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

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 (14), will yield the mean residence time. This is most easily accomplished by using the table created in step 3 above (Table 4), which facilitates the necessary calculations. Time is recorded in equally spaced increments. If discharge was constant during the period of tracer recovery, then the $Q$ column (column 3) of the table has a

constant value as well. The $C \times Q$ column (column 5) is obtained from the product of the third and fourth column values. The $t \times C \times Q$ column (column 6) is obtained from the product of the $C \times Q$ column with the $t$ column (column 1), and by applying all necessary conversions (*e.g.*, hours vs. seconds).

5. **Calculate Tracer Mass Recovery** When the table of values is complete, Equation (11) can be solved by summing column 5 and multiplying by a time conversion to get units of mass only. Hence, the solution to Equation (11) is acquired in a simplified manner by

$$M_O = \int\limits_0^\infty Q(t)C(t)dt \approx \sum_{i=1}^n Q_i C_i \Delta t_i \approx t_c \sum_{i=1}^n (Q_i C_i) \qquad (69)$$

where $t_c$ is any necessary time conversion factor that allows for units of mass.

6. **Calculate Mean Tracer Residence Time** Mean tracer residence time $\bar{t}$ is found by solving Equations (14) and (17). Equations (14) and (17) are solved by the same method that Equation (11) is solved; by simplified summation of the data. Using Table 4, summing column 6, and multiplying 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. **Calculate Longitudinal Dispersion** If the method of moments is used to solve for longitudinal dispersion the basics of steps 3 and 4 above are repeated to create Table 5. Columns 4 and 5 are again summed and the results converted to appropriate units. Then Equations (29) and (30) are applied depending on the type of tracer release. Alternatively, if the Chatwin method is used, Table 6 is set up using legitimate values

Table 5. Table representing tracer recovery data for processing.

| Sample | $(t-\bar{t})^2$ $(\mathrm{T}^2)$ | $Q$ $(\mathrm{L}^3\ \mathrm{T}^{-1})$ | $C$ $(\mathrm{M}\ \mathrm{L}^{-3})$ | $C \times Q$ $(\mathrm{M}\ \mathrm{T}^{-1})$ | $(t-\bar{t})^2 \times C \times Q$ $(\mathrm{M}\ \mathrm{T})$ |
|---|---|---|---|---|---|
| ... | ... | ... | ... | ... | ... |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| ... | ... | ... | ... | ... | ... |

for time $(0 < t_\kappa \leq x_s/\bar{v})$, and solved parameters for $b_i$ (Equation [40]) representing the Chatwin designation. A straight line is then drawn through the legitimate values, and longitudinal dispersion is solved using either Equation (41) or (42).

Table 6. Table representing Chatwin values.

| Sample | Time (h) | Chatwin $(s^{1/2})$ | Fit $(s^{1/2})$ | Residual (dimen.) |
|--------|----------|---------------------|-----------------|-------------------|
| ... | ... | ... | ... | ... |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| ... | ... | ... | ... | ... |

9. **Repeat for Subsequent Sampling Stations** Repeat the above steps for all wells and/or springs in which the tracer was recovered.

10. **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.

11. **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 the result by 100.

12. **Calculate Additional Parameters** Calculate the Péclet number, Reynolds number, *etc.* as desired and appropriate, using the equations developed in Section 3. on page 26

## 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 over a period of 24 minutes (0.4 hour) at the RCA del Caribe (Barceloneta, Puerto Rico) Superfund site for a tracing study. Injection occurred at a rate of 13.75 gpm ($8.78 \times 10^{-4}$ m$^3$ s$^{-1}$) at 940 feet (287 m) below land surface (BLS), which is also below the confining layer for the bottom of the shallow aquifer.

The leakage rate from the deep aquifer up the annular space to the shallow aquifer was 450 gpm. The total height that the tracer needed to rise to reach the shallow aquifer was 240 feet (73 m) or 700 feet (213 m), BLS. The time down the well (940 feet) was 11.18 minutes, and the rise up the annular space 240 feet was 1.08 minutes for a total reduction

of the time of travel by 12.26 minutes (0.2 hour), and a consequent increase in the flow velocity according to Equation (2).

Recovery was at an observation well 110 feet (34 meters) from the injection well that was pumped at a constant rate of 6.0 gpm ($3.79 \times 10^{-4}$ m$^3$ s$^{-1}$). Figure 13 displays the BTC for the RCA del Caribe Superfund site, and Table 7 (slightly modified from 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 (11) or, more simply, by Equation (69). Equation (69) 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 6 of Table 7 lists the products of columns 4 and 5 and is summed at the end.

The summed results of column 6 of Table 7 must be multiplied by 3,600 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 (69) is not as precise as Equation (11). However, results obtained by Equation (69) 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 (14) or its equivalent discrete form. This is accomplished by multiplying column 6 by column 3 in Table 7, and recording the results in column 7.  Summing column 7 of Table 7, and multiplying by 3,600 seconds will yield results in units of mass–time

$$
\left(1.54 \times 10^7 \text{ mg}\right)\left(3.60 \times 10^3 \text{ s}\right) = 5.54 \times 10^{10} \text{mg s}
$$

RCA.DAT
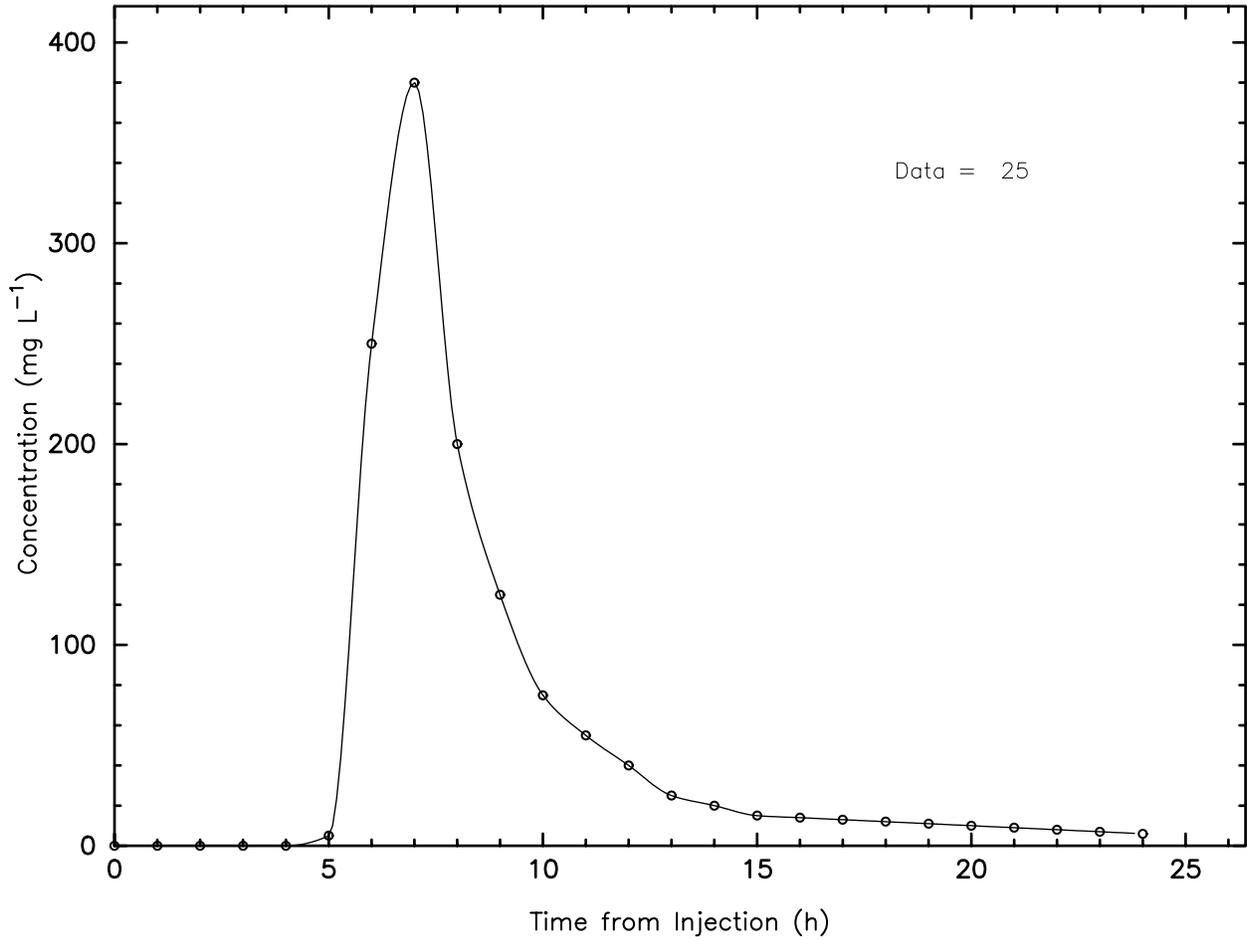


Figure 13. Tracer-breakthrough curve for the RCA de Caribe Superfund site.

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Table 7. Discharge values and tracer recovery values at specific times.

| Sample | $t$ (h) | $Q$ (m$^3$ s$^{-1}$) | $C$ (mg m$^{-3}$) | $C \times Q$ (mg s$^{-1}$) | $t \times C \times Q$ (mg) |
|--------|---------|---------------------|-------------------|----------------------------|----------------------------|
| 1  | 0.00  | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 2  | 1.00  | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 3  | 2.00  | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 4  | 3.00  | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 5  | 4.00  | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 6  | 5.00  | $3.79 \times 10^{-4}$ | $5.00 \times 10^3$ | $1.89 \times 10^0$ | $3.41 \times 10^4$ |
| 7  | 6.00  | $3.79 \times 10^{-4}$ | $2.50 \times 10^5$ | $9.46 \times 10^1$ | $2.04 \times 10^6$ |
| 8  | 7.00  | $3.79 \times 10^{-4}$ | $3.80 \times 10^5$ | $1.44 \times 10^2$ | $3.63 \times 10^6$ |
| 9  | 8.00  | $3.79 \times 10^{-4}$ | $2.00 \times 10^5$ | $7.57 \times 10^1$ | $2.18 \times 10^6$ |
| 10 | 9.00  | $3.79 \times 10^{-4}$ | $1.25 \times 10^5$ | $4.73 \times 10^1$ | $1.53 \times 10^6$ |
| 11 | 10.00 | $3.79 \times 10^{-4}$ | $7.50 \times 10^4$ | $2.84 \times 10^1$ | $1.02 \times 10^6$ |
| 12 | 11.00 | $3.79 \times 10^{-4}$ | $5.50 \times 10^4$ | $2.08 \times 10^1$ | $8.25 \times 10^5$ |
| 13 | 12.00 | $3.79 \times 10^{-4}$ | $4.00 \times 10^4$ | $1.51 \times 10^1$ | $6.54 \times 10^5$ |
| 14 | 13.00 | $3.79 \times 10^{-4}$ | $2.50 \times 10^4$ | $9.46 \times 10^0$ | $4.43 \times 10^5$ |
| 15 | 14.00 | $3.79 \times 10^{-4}$ | $2.00 \times 10^4$ | $7.57 \times 10^0$ | $3.82 \times 10^5$ |
| 16 | 15.00 | $3.79 \times 10^{-4}$ | $1.50 \times 10^4$ | $5.68 \times 10^0$ | $3.07 \times 10^5$ |
| 17 | 16.00 | $3.79 \times 10^{-4}$ | $1.40 \times 10^4$ | $5.30 \times 10^0$ | $3.05 \times 10^5$ |
| 18 | 17.00 | $3.79 \times 10^{-4}$ | $1.30 \times 10^4$ | $4.92 \times 10^0$ | $3.01 \times 10^5$ |
| 19 | 18.00 | $3.79 \times 10^{-4}$ | $1.20 \times 10^4$ | $4.54 \times 10^0$ | $2.94 \times 10^5$ |
| 20 | 19.00 | $3.79 \times 10^{-4}$ | $1.10 \times 10^4$ | $4.16 \times 10^0$ | $2.85 \times 10^5$ |
| 21 | 20.00 | $3.79 \times 10^{-4}$ | $1.00 \times 10^4$ | $3.79 \times 10^0$ | $2.73 \times 10^5$ |
| 22 | 21.00 | $3.79 \times 10^{-4}$ | $9.00 \times 10^3$ | $3.41 \times 10^0$ | $2.58 \times 10^5$ |
| 23 | 22.00 | $3.79 \times 10^{-4}$ | $8.00 \times 10^3$ | $3.03 \times 10^0$ | $2.40 \times 10^5$ |
| 24 | 23.00 | $3.79 \times 10^{-4}$ | $7.00 \times 10^3$ | $2.65 \times 10^0$ | $2.19 \times 10^5$ |
| 25 | 24.00 | $3.79 \times 10^{-4}$ | $6.00 \times 10^3$ | $2.27 \times 10^0$ | $1.96 \times 10^5$ |
| | | | $\sum_{i=1}^{n}$ | $4.85 \times 10^2$ | $1.54 \times 10^7$ |

Note: "Sample" arbitrarily assumes that the first sample was collected at the time of injection.

Time $t$ is listed here in hours, but is converted to seconds before multiplying with $C$ and $Q$.

(source: RCA, 1992)

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

$$\frac{5.54 \times 10^{10} \text{ mg s}}{1.75 \times 10^6 \text{ mg}} = 3.17 \times 10^4 \text{ s}$$

$$= 8.79 \times 10^0 \text{ h}$$

This is necessarily corrected for time to reach the flow zone ($t_{inf} = 0.2$ h)

$$8.79 \times 10^0 \text{ h} - 2.0 \times 10^{-1} \text{ h} = 8.59 \times 10^0 \text{ h}$$

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 (25) or, more simply, by dividing the distance to the sampling station by the time of travel, minus one half the pulse-injection time, which is a modification of Equation (2)

$$\frac{34 \text{ m}}{(8.79 \text{ h} - 0.2 \text{ h}) - \frac{0.4}{2} \text{ h}} = 4.05 \times 10^0 \text{ m h}^{-1}$$

$$= 1.13 \times 10^{-3} \text{ m s}^{-1}$$

This may then be 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.

The difference between the perceived velocity and the actual velocity may then be obtained from Equation (3)

$$\frac{34 \text{ m} (0.2 \text{ h})}{(8.79 \text{ h} - 0.2 \text{ h}) \, 8.79 \text{ h}} = 9.22 \times 10^{-2} \text{ m h}^{-1}$$

which suggests a relatively insignificant difference of 0.1 m h$^{-1}$ for this example.

### 4.1.4.  Longitudinal Dispersion Example

Longitudinal dispersion is most accurately estimated by the Chatwin method (Equation [31]), which can be tedious. Using just the first valid time value, Equation (40) appears as

$$b_i = \sqrt{1.80 \times 10^4 \ln\left(\frac{3.80 \times 10^5 \sqrt{2.52 \times 10^4}}{5.0 \times 10^3 \sqrt{1.80 \times 10^4}}\right)} = 284.57 \text{ s}^{1/2}$$

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Table 8. Chatwin parameter values for the RCA data set.

| Sample | Time (h) | Chatwin ($s^{1/2}$) | Fit ($s^{1/2}$) | Residual (dimen.) |
|--------|----------|---------------------|-----------------|-------------------|
| 6      | 5.0      | 284.57              | 266.33          | 18.24             |
| 7      | 6.0      | 103.48              | 132.01          | -28.52            |
| 8      | 7.0      | 0.00                | -2.32           | 2.32              |
| 9      | 8.0      | -128.70             | -136.65         | 7.96              |
| 10     | 9.0      | -178.75             | -270.98         | 92.23             |
| 11     | 10.0     | -228.03             | -405.31         | 177.28            |
| 12     | 11.0     | -259.98             | -539.64         | 279.66            |
| 13     | 12.0     | -292.60             | -673.97         | 381.37            |
| 14     | 13.0     | -335.96             | -808.30         | 472.33            |
| ⋮      | ⋮        | ⋮                   | ⋮               | ⋮                 |
| 25     | 24.0     | -552.44             | -2285.91        | 1733.47           |

after converting the time and concentration values to consistent values (seconds and mg m$^{-3}$ [$\mu$ L$^{-1}$], respectively for this example). Partial results for the RCA example data set are shown in Table 8. Samples collected prior to $t = 5.0$ hours were devoid of tracer ($C = 0.0$ mg L$^{-1}$), so the first legitimate sample for consideration for the Chatwin analysis occurs at 5.0 hours. According to the limit $t_\kappa \leq 8.40$ h (see Section 3.3.2. on page 34), only samples 6–9 listed in Table 8 are considered valid for the Chatwin analysis (assuming that sample 1 [Table 4] represents time zero). A casual inspection of Table 8 will indicate that residual errors (Chatwin value minus the Fit value) after sample 9 become increasingly large further indicating the inappropriateness of samples 10–25.

Also, it should be noted that while time values listed in Table 8 are in hours, the Chatwin and Fit values are listed in seconds to the one-half power. The Fit values are obtained by fitting a straight line through the Chatwin values plotted against time. The choice of units does not matter provided, appropriate corrections are made to the final dispersion estimates.

Using samples 6–9, longitudinal dispersion by the Chatwin method is $D_L = 1.15$ m$^2$ h$^{-1}$ and a corresponding Péclet number is obtained from Equation (56)

$$P_e = \frac{34\,(4.05)}{1.15} = 120.74$$

If the method of moments are used to solve for longitudinal dispersion (Equation [30]), then

$$D_L = \left(12.75 - \frac{0.4}{12}\right)\left[\frac{(4.05)^3}{2\,(34)}\right] = 12.42 \text{ m}^2 \text{ h}^{-1}$$

where $\sigma_t^2 = 12.75$ hours was obtained from Equation (17) in summation form (Table 9) similar to the method used to obtain the mean resident time (Table 7).

As with Table 7, column 5 in Table 9 is multiplied by column 2 in Table 9 and the results recorded in column 6. Summing column 6 of Table 9 and multiplying by 3,600 seconds will yield results in units of mass–time

$$\left(2.23 \times 10^7 \text{ mgs}\right)\left(3.60 \times 10^3 \text{ s}\right) = 8.03 \times 10^{10} \text{mg s}^2$$

Dividing by the mass recovered (1.75 kg) will yield the time of travel variance of the tracer in units of time.

$$\frac{8.03 \times 10^{10} \text{ mg s}^2}{1.75 \times 10^6 \text{ mg}} = 4.59 \times 10^4 \text{ s}^2$$
$$= 12.75 \times 10^0 \text{ h}^2$$

The Péclet number is now obtained as $P_e = 11.09$.

### 4.1.5. System Volume

The flow system volume may be estimated using Equation (47). The average discharge for the RCA del Caribe site, $3.79 \times 10^{-4}$ m$^3$ s$^{-1}$ (6 gpm), is multiplied by the mean residence time, $3.09 \times 10^4$ s, to obtain the system volume.

$$\left(3.79 \times 10^{-4} \text{ m s}^{-1}\right)\left(3.09 \times 10^4 \text{ s}\right) = 1.17 \times 10^1 \text{ m}^3$$

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.

Table 9. Table of values used to determine the time of travel variance.

| Sample | $(t - \bar{t})^2$ (h²) | $Q$ (m³ s⁻¹) | $C$ (mg m⁻³) | $C \times Q$ (mg s⁻¹) | $(t - \bar{t})^2 \times C \times Q$ (mg s) |
|---|---|---|---|---|---|
| 1 | $7.40 \times 10^1$ | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 2 | $5.78 \times 10^1$ | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 3 | $4.36 \times 10^1$ | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 4 | $3.14 \times 10^1$ | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 5 | $2.12 \times 10^1$ | $3.79 \times 10^{-4}$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ | $0.00 \times 10^0$ |
| 6 | $1.30 \times 10^1$ | $3.79 \times 10^{-4}$ | $5.00 \times 10^3$ | $1.89 \times 10^0$ | $8.85 \times 10^4$ |
| 7 | $6.79 \times 10^0$ | $3.79 \times 10^{-4}$ | $2.50 \times 10^5$ | $9.46 \times 10^1$ | $2.31 \times 10^6$ |
| 8 | $2.58 \times 10^0$ | $3.79 \times 10^{-4}$ | $3.80 \times 10^5$ | $1.44 \times 10^2$ | $1.33 \times 10^6$ |
| 9 | $3.66 \times 10^{-1}$ | $3.79 \times 10^{-4}$ | $2.00 \times 10^5$ | $7.57 \times 10^1$ | $9.97 \times 10^4$ |
| 10 | $1.56 \times 10^{-1}$ | $3.79 \times 10^{-4}$ | $1.25 \times 10^5$ | $4.73 \times 10^1$ | $2.66 \times 10^4$ |
| 11 | $1.95 \times 10^0$ | $3.79 \times 10^{-4}$ | $7.50 \times 10^4$ | $2.84 \times 10^1$ | $1.99 \times 10^5$ |
| 12 | $5.74 \times 10^0$ | $3.79 \times 10^{-4}$ | $5.50 \times 10^4$ | $2.08 \times 10^1$ | $4.30 \times 10^5$ |
| 13 | $1.15 \times 10^1$ | $3.79 \times 10^{-4}$ | $4.00 \times 10^4$ | $1.51 \times 10^1$ | $6.28 \times 10^5$ |
| 14 | $1.93 \times 10^1$ | $3.79 \times 10^{-4}$ | $2.50 \times 10^4$ | $9.46 \times 10^0$ | $6.58 \times 10^5$ |
| 15 | $2.91 \times 10^1$ | $3.79 \times 10^{-4}$ | $2.00 \times 10^4$ | $7.57 \times 10^0$ | $7.93 \times 10^5$ |
| 16 | $4.09 \times 10^1$ | $3.79 \times 10^{-4}$ | $1.50 \times 10^4$ | $5.68 \times 10^0$ | $8.36 \times 10^5$ |
| 17 | $5.47 \times 10^1$ | $3.79 \times 10^{-4}$ | $1.40 \times 10^4$ | $5.30 \times 10^0$ | $1.04 \times 10^6$ |
| 18 | $7.05 \times 10^1$ | $3.79 \times 10^{-4}$ | $1.30 \times 10^4$ | $4.92 \times 10^0$ | $1.25 \times 10^6$ |
| 19 | $8.83 \times 10^1$ | $3.79 \times 10^{-4}$ | $1.20 \times 10^4$ | $4.54 \times 10^0$ | $1.44 \times 10^6$ |
| 20 | $1.08 \times 10^2$ | $3.79 \times 10^{-4}$ | $1.10 \times 10^4$ | $4.16 \times 10^0$ | $1.62 \times 10^6$ |
| 21 | $1.30 \times 10^2$ | $3.79 \times 10^{-4}$ | $1.00 \times 10^4$ | $3.79 \times 10^0$ | $1.77 \times 10^6$ |
| 22 | $1.54 \times 10^2$ | $3.79 \times 10^{-4}$ | $9.00 \times 10^3$ | $3.41 \times 10^0$ | $1.88 \times 10^6$ |
| 23 | $1.79 \times 10^2$ | $3.79 \times 10^{-4}$ | $8.00 \times 10^3$ | $3.03 \times 10^0$ | $1.96 \times 10^6$ |
| 24 | $2.07 \times 10^2$ | $3.79 \times 10^{-4}$ | $7.00 \times 10^3$ | $2.65 \times 10^0$ | $1.98 \times 10^6$ |
| 25 | $2.37 \times 10^2$ | $3.79 \times 10^{-4}$ | $6.00 \times 10^3$ | $2.27 \times 10^0$ | $1.94 \times 10^6$ |
| | | | $\sum_{i=1}^{n}$ | $4.85 \times 10^2$ | $2.23 \times 10^7$ |

Note: "Sample" arbitrarily assumes that the first sample was collected at the time of injection.

Time $(t - \bar{t})^2$ is listed here in hours², but is converted to seconds² before multiplying with $C$ and $Q$.

# 5. QTRACER2 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 CD 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 data points. 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 has 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 BTCs, 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 data point for extrapolation. This is achieved by using the entire BTC 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. 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 achieved by projecting data for the decreasing limb of the BTC 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 is 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 are decreasing, then the extrapolated discharge data will increase to one-half the original decreasing value. If the measured discharge data are 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 Equations (29) and (30). Using Equations (29) or (30) 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 QTRACER2 and may be analyzed according to the method described by Mull *et al.* (1988). The discussion by Mull *et al.* is very comprehensive and, therefore, 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 tracing site (1) may have multiple discharge locations, many of which may not be continuously monitored for tracer; and (2) may require more quantitative tracing experiments than can be reasonably undertaken.

## 5.5.  RANGE OF POSSIBILITIES OF QTRACER2

QTRACER2 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.

QTRACER2 was initially designed to be used in karst systems primarily, but it will handle any other typical hydrological system (*e.g.*, fractured-rock systems) reasonably

well when told to do so in the sampling station data file. It may be used to evaluate BTCs 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 when the output data make sense. By exercising some basic judgment, QTRACER2 can be effectively used in a variety of environments.

## 5.6.  COMPUTER GRAPHICS

A high-quality color graphics algorithm, PGPLOT[1] (Pearson, 1997), that allows cascading of graphics screens, direct printing, creation of screen files, *etc.*, using pull-down menus in the Windows environment has been included in QTRACER2. (The original interactive capabilities developed by Kahaner and Anderson (1990), and utilized in QTRACER are no longer available.) The graphics routine used here also 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 any type of printer is possible.

### 5.6.1.  Features of the Interactive Graphics Loop

Running QTRACER2 starts a conventional Windows screen with a series of pull-down menus (Table 10). Each underlined character in Table 10 indicates that the Alt key plus the underlined character implements the respective menu item. For example, `Alt+F` initiates the pull-down menu items underneath the File heading. Of course, the mouse pointer can be used to access the menu items.

It is necessary to point out here that most users will not use the pull-down menus often. Most of the more useful graphics functions have been built directly into QTRACER2 to alleviate excess work by the user. However, in some instances, the user may find the functions of value. For example, selecting the Cascade function under the Window pull-down menu after a total five or six graphics plots have been produced in a series of child-windows, will cause the child-windows to stack, slightly offset to the lower right.

---

[1]PGPLOT may be obtained from http://www.astro.caltech.edu/~tjp/pgplot/

Table 10. Pull-down menu items available in QTRACER2.

| File | Edit | View | State | Window | Help |
|------|------|------|-------|--------|------|
| Print... | Select Text | Size To Fit | Pause Ctrl+S | Cascade | Contents |
| Save... | Select Graphics | Full Screen Alt Enter | | Tile | Using Help |
| Exit Ctrl+C | Select All | | | Arrange Icons | About |
| | Copy Ctrl+Ins | | | Iput | |
| | Paste | | | Clear Paste | |
| | | | | Status Bar | |
| | | | | 1Graphic 1 | |
| | | | | 2PGPlot Graphics, # 1 | |
| | | | | ⋮ | |

**File** Items listed under this heading are described as follows.

**Print...** *A screen dump to the local printer attached to the respective PC.*

**Save...** *Save the screen as a bitmapped (\*.BMP) file.*

**Exit Ctrl+C** *Exit the program.*

---

**Edit** Items listed under this heading are described as follows.

**Select Text** *Select text for pasting to the clipboard.*

**Select Graphics** *Select graphics for pasting to the clipboard.*

**Select All** *Select both text and graphics for pasting to the clipboard.*

**CopyC trl+Ins** *Copy selected items to the clipboard.*

**Paste** *Paste selected items to the screen.*

---

**View** Items listed under this heading are described as follows.

**Size To Fit** *Fit the graphics screen to the view surface without scroll bars.*

**Full ScreenAlt+En ter** *Fit the entire graphics screen to the view surface without the menu items displayed (a left-mouse click returns to the original screen).*

---

**State** Items listed under this heading are described as follows.

**Pause Ctrl+S** *Pause the graphic display.*

**Resume Ctrl+Q** *Resume graphic display.*

The two items Pause and Resume appear only as alternates of each other so that only the one that is not currently functioning is accessible. The item that is currently in operation is not displayed in the pull-down menu.

---

**Window** Items listed under this heading are described as follows.

**Cascade** *Allows for a cascading view of multiple child windows at one time.*

**Tile** *Allows for a tile display of multiple child windows at one time.*

**Arrange Icons** *Not currently used in* QTRACER2.

**Input** *Automatically displays the input screen* (Graphic 1) *for data input.*

**Clear Paste** *Clears an item pasted onto the screen.*

**Status Bar** *Displays the current operating mode of the displayed graphics screen in a bar at the bottom of the screen (when "check marked").*

**1 Graphic 1** *Name of the data input screen ("check marked") if active.*

**2 PGPlot Graphics, # 1** *Identifying name/number of all subsequently opened graphics screens (active when "check marked").*

**Help** Items listed under this heading are described as follows.

**Contents** *Listing of available help contents.*

**Using Help** *Describes the use of the Help function.*

**About** *Identifies the current version of* QTRACER (Version 2.0).

## 5.7. QTRACER2 SOURCE

The FORTRAN source for QTRACER2 is included on the CD. It is a very large program that had to be split into pieces to allow its use on a PC. It is not recommended that users attempt to follow the logic or modify the program. Questions regarding the program's functioning can be addressed to the author.

In addition, the graphics routine developed at the California Institute of Technology is included. This program is not allowed for use for commercial products.

# 6. USING QTRACER2

The QTRACER2 program for BTC analysis is an easy-to-use computer package that requires little more from the user than pressing `<ENTER>` when requested or manipulating pull-down menus with a mouse. However, QTRACER2 does require creating data-input files first for processing. Using data-input files rather than requiring interactive responses to questions posed by the program facilitates more rapid data processing while minimizing the opportunities for incorrect data entry.

## 6.1. QTRACER2 PROGRAM AND EXAMPLE DATA FILES

Before running the program, the user should copy all QTRACER2 files to the hard drive and put the supplied CD-ROM disk in a safe place. Although the CD-ROM has plenty of storage space for the creation of data-output files and graphics files, the possibility of damage to the QTRACER2 program file from excess use cannot be ignored.

### 6.1.1. Loading QTRACER2 and Example Data Files

1. After "booting" up the computer, place the CD-ROM into the CD-ROM drive.

2. At the computer "desk top" place the mouse pointer (arrow) on the "My Computer" icon and click the *Right* mouse button *(Right Click)*.

3. *Left Click* on the word "Explore" in the pop-up menu. Alternatively, just press the letter "`E`" on the keyboard.

4. Place the mouse pointer on the CD-ROM drive icon (*e.g.*, `D:` or `E:`) and *Left Double-Click*.

5. *Left Click* "Edit" at the top of the Window Screen and *Left Click* on "Select All" in the pull-down menu. Alternatively, just press the letter "`A`" on the keyboard.

6. *Left Click* on the "Copy" icon on the "Tool Bar" near the top of the Window Screen (second row). Alternatively, *Left Click* on "Edit" at the top of the Window Screen and then *Left Click* on "Copy" or just press "`C`" on the keyboard.

7. *Left Click* on the preferred hard drive (*e.g.*, `C:`).

8. *Left Click* on the "Paste" icon on the "Tool Bar" near the top of the Window Screen (second row). Alternatively, *Left Click* on "Edit" at the top of the Window Screen and then *Left Click* on "<u>P</u>aste" or just press "P" on the key board.

A Folder named Qtracer2 will be created on the chosen hard drive and all the appropriate files copied accordingly to the appropriate file folders[2].

## 6.2.   QTRACER2 EXECUTION

QTRACER2 is very easy to use. Once the appropriate data files are created (which are nearly self-explanatory) QTRACER2, for the most part, requires nothing more than pressing the `<ENTER>` (`<RETURN>`) key as requested or manipulation of the mouse and clicking with the left-mouse button.

1. In Windows Explorer, *Left Double-Click* the QTRACER2 folder and then *Left Double-Click* the QTR.EXE file which will initiate program operation.[3]

2. The program prompts the user to enter the file to be evaluated (unless a file was specified when starting the program using a DOS prompt). Press `<ENTER>` to automatically run the default file, `QTRACER.D`, which calls `QTRACER.DAT` (these two files correspond with ATKIN.D and ATKIN.DAT from the original QTRACER Version 1.0, respectively). However, if the data files are in different locations from QTRACER2, the user must provide the correct path to the `*.D` and `*.DAT` files. One advantage of creating a subdirectory on the hard disk is that the program will find all files automatically because they are all at the same location as the executable file.

---

[2]The first version of Qtracer was designed for MSDOS®use and required that the files be moved according to the following instructions which may still be used:

- At the `C:\>` prompt, type "`MKDIR QTRACER2`" (without the quotes — whenever quotes appear in this section type the requested information without the quotes).

- Next copy the executable and data files stored in the file Qtr_dos on the CD to your hard disk. For example, you might type (if C is your disk drive): "`COPY D:\*.* C:\QTRACER2\*.*`."

- Repeat the above commands for the other files on the CD.

- Put your CD in a safe location.

[3]If a command prompt is preferred then at the `C:\>` prompt, type "`CD\QTRACER2`" without the quotes. The user will then see a new prompt; `C:\QTRACER2>`. Assuming the user also copied the necessary data files or created your own, the user may now type "`QTR`" to run the program by responding to the requested information. The user may want to type "`QTR` *filename*" such as "`QTR QTRACER.D`", which will automatically load and run the Atkinson data set described in the journal article (Field and Nash, 1997). The user may do the same with the Mull *et al.* (1988) data by typing "`QTRACER2 MULL.D`" to load the appropriate data files and begin processing.

Additional information regarding QTRACER2 execution is presented in Section 7. on page 90 However, the really important information (files creation) is listed in this section.

## 6.3.  QTRACER2 FUNCTIONING

QTRACER2 runs by processing two types of files at once. The first file processed is a header file, which identifies the amount of tracer injected into the hydrologic system 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 must include all necessary information for the program to run. They also allow the user to run the program without interaction with the user (batch mode), pause processing to allow the user to observe numerical output, and display high-quality graphics. What follows are seven sets of data files that may be used to test the QTRACER2 program. The data files may also be reviewed directly, as they are simple ASCII files.

Run QTRACER2 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) [`QTRACER.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.

## 6.4.  SAMPLE FILES ON DISK

The following nine "header" data files (`*.D`) and their respective sample station data files (`*.DAT`) are included on the disk (Table 11). Each header file must reference at least one corresponding sample station data file. However, the number of sample station data files that correspond to a header file is limited only by your computer's capabilities.

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

Descriptions of data files listed in Table 11 follow.

1. `QTRACER.D` and `QTRACER.DAT` are hypothetical data sets provided by Dr. Timothy Atkinson (Atkinson, 1987) for educating students (of which this author was one) on the proper methodology for analyzing and interpreting BTCs. Analysis of these data sets using QTRACER2 is presented in considerable detail in Field and Nash (1997).

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Table 11. Example data files on disk.

| Header Data File | Sample Station Data File |
| --- | --- |
| QTRACER.D | QTRACER.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 |
| UVAS281.D | UVAS281.DAT |
| MOBILE.D | MOBILE.DAT |

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 BTC 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 that QTRACER2 allows for and corrects. Analysis of these data sets using QTRACER2 is presented in considerable detail in Field and Nash (1997).

3. `LOST.D` and `LOST.DAT` are data sets listing the results of a BTC. They were generated by the senior author (and other students) when Dr. Atkinson was instructing proper methodology for conducting tracer tests and analyzing and 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 QTRACER2. 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. on page 50 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) that serve to demonstrate that an "ideal" BTC is not necessary for QTRACER2 to function

properly. The Toplita data sets are also excellent for demonstrating QTRACER2's data extrapolation capabilities because of the shape of the curve and the position of the last measured data point.

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 10.1. on page 154 for a description of NDATA). A deliberately "huge" data set was constructed to demonstrate QTRACER2'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 QTRACER2's capabilities of handling "huge" data sets, but with a "variable" discharge (`GAR2.DAT` has a constant discharge).

8. `UVAS281.D` and `UVAS281.DAT` consists of original surface-water tracing data published by Zand *et al.* (1976) and republished in Bencala and Walters (1983). It is available from the U.S. Geological Survey and is provided here to illustrate QTRACER2's ability to evaluate surface-water tracing data (see Section 8. on page 115).

9. `MOBILE.D` and `MOBILE.DAT` consists of slightly modified data from Molz *et al.* (1986a,b). It is reprinted here to illustrate QTRACER2's ability to evaluate tracer tests conducted in porous media (see Section 8. on page 115).

**NOTE**: EDIT ONE OF THE *.D FILES AND SAVE AS A NEW FILE WITH A NEW FILE NAME. THEN EDIT ONE OF THE *.DAT FILES AS OFTEN AS NECESSARY FOR EACH SAMPLING STATION TO BE ANALYZED. SAVE EACH *.DAT FILE AS A NEW FILE WITH A NEW FILE NAME.

## 6.5. DESCRIPTION OF *.D FILES

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

A *.D file (*e.g.*, `QTRACER.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.

```
QUANTITY OF TRACER INJECTED
450
UNITS OF MEASURE (1-lbs, 2-kg, 3-g, 4-mg)
3
TYPE OF RELEASE AND TIME FOR RELEASE (1-impulse, 2-pulse, 3-step) [HOURS]
1 0.0
TIME FOR TRACER TO REACH FLOW ZONE [HOURS]
0.0
SAMPLING DATA FILES LIST
QTRACER.DAT
```

Figure 14. `QTRACER.D` header file for QTRACER2 processing.

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 on the next line the user enters the appropriate response that QTRACER2 will read. 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 system. For the `QTRACER.D` example `450` is listed by the user because this was the hypothetical tracer quantity injected into the system.

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 parentheses represent the valid units allowed by QTRACER2. The user responds with the appropriate units. For the `QTRACER.D` example the number `3` is listed to indicate grams (g) as the unit of measure.

Next is a request for a brief description of the type and time required for tracer injection.

```
TYPE OF RELEASE AND TIME FOR RELEASE (1-impulse, 2-pulse, 3-step) [HOURS]
1 0.0
```

The numbers enclosed in parentheses represent valid choices for the type of injection used

for the tracer test where impulse represents an instantaneous injection, pulse represents an injection that occurred over some period of measurable time, and step represents a continuous injection for the length of the tracer test period. The listed units [HOURS] is a required entry only for a pulse and step (continuous) releases. An impulse release demands that the time for release be left blank or set to zero; anything greater than zero will precipitate QTRACER2 resetting the release time to zero.

The file now requires some entry for the time taken to reach the flow zone. `TIME FOR TRACER TO REACH FLOW ZONE [HOURS]`
`0.0`
Typically this value will be zero, which must be entered (not left blank) for QTRACER2 to properly function. The importance of this value is described by Equations (2) and (3) and is used to properly determine $\bar{t}$, $\bar{upsilon}$, and $D_{x_s}$.

Lastly, the program asks for the name of all subfiles to be called by QTRACER2 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.*, `QTRACER.DAT`). The subfiles correspond to each sampling station at which tracer was recovered.

`SAMPLING DATA FILES LIST`
`QTRACER.DAT`
For the `QTRACER.D` example, only one station is listed as having recovered tracer, `QTRACER.DAT`, because that is the only station at which this hypothetical trace recovered the tracer.

However, if 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 `QTRACER.D` tracer test might be listed as:

```
QTRACER.1
QTRACER.2
QTRACER.3
   .
   .
   .
QTRACER.23
```
Any other appropriate names such as the names of various monitoring wells or monitored springs are acceptable. The only requirement is that the user be able to recognize the names after QTRACER2 has been run, as it is most advantageous to run QTRACER2 in batch mode for large data sets.

## 6.6.  DESCRIPTION OF *.DAT FILES

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

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

### 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. The first item for a *.DAT file 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.
**<u>NOTE</u>**: `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 `QTRACER.DAT` example, 3 was recorded because tracer concentration is recorded at the end of this file (corresponding to time data) in units of $\mu$g 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 QTRACER2 how to respond. The number 0 for the `QTRACER.DAT` data set tells QTRACER2 that no value for background is available — no "value" is required. The number 1 tells QTRACER2 that a background value is available for subtracting from the data set — a number 1 *MUST* be

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```
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 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 0
ESTIMATE SYSTEM 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=1.0]
1 1.5
FLOW MEDIUM: POROSITY (1=subsurface channel, 2=surface channel,
        3=porous medium, 4=fractured medium) [VALUE, def=1.0]
1 1.0
IF POROUS FLOW: UNITS, HYDR. COND. (1=m/s, 2=m/hr, 3=ft/s, 4=m/hr, 0=null)
IF FRACTURE(S) FLOW: UNITS, HEIGHT (1=m, 2=ft, 0=null) [VALUE]
0 0.0
NAME OF THE FILE OF INPUT/OUTPUT VALUES
Q1.OUT
INTERPOLATE DATA (1=yes, 0=no) [NUMBER OF KNOTS]
0 1000
NAME OF THE INTERPOLATED OUTPUT VALUES FILE
Q1.INT
```

Figure 15. `QTRACER.DAT` sampling station data file for QTRACER2 processing.

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```
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 PRINT PLOT OPLOT)
0 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\Q1.ADV
FLAG FOR NORMALIZED CONCENTRATION VALUES FILE (1/0)
1
NAME OF FILE FOR NORMALIZED CONCENTRATION VALUES (VALID IF FLAG=1)
Q1.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)
Q1.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)
Q1.STN
VISUALIZATION: STANDARDIZED TIME AND CONCENTRATION (CHECK PLOT JOIN OPLOT)
0 0 1 0
```

Figure 15.  `QTRACER.DAT` sampling station data file for QTRACER2 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.  `QTRACER.DAT` sampling station data file for QTRACER2 processing (continued).

followed by a number [VALUE] (*i.e.*, concentration) in the *SAME* units as those in which 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 only if appropriate. However, this number may be zero.

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 $\mu$g 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 $\mu$g 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. QTRACER2 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, the value for which must be included in the next section with the discharge units of measure. So for the QTRACER.DAT file, a variable discharge 1 is listed, which means that there *MUST* be a third column of data at the end of the QTRACER.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, QTRACER2 needs to know in which units discharge was measured so that an appropriate correction to allow for consistent units can be made. A considerable range of discharge unit measures is allowed by QTRACER2, 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 for which are listed at the end of the data file (`QTRACER.DAT`). (QTRACER2 converts all other discharge choices to m$^3$ s$^{-1}$ prior to processing the file.)

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.  System Volume

The system volume can be estimated by QTRACER2 provided the time-concentration data file *begins* at zero time. (QTRACER2 now automatically adds zero time when zero time is absent from the time-concentration data file.) A simple on/off switch informs QTRACER2 to estimate volume. If the switched is set to off, then subsequent geometries (*e.g.*, cross-sectional area) will also not be estimated.

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

The switch value `1` for the `QTRACER.DAT` example informs QTRACER2 that system volume should be estimated.

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### 6.6.7. Radial Distance

QTRACER2 needs to know the straight-line distance to the sampling station from the injection site and the units by which distance 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 `QTRACER.DAT` example.

### 6.6.8. Correction for Sinuosity

Because most solution conduits and fractures are not straight-line features, a sinuosity factor may be included for QTRACER2 to use in processing the data.

```
CORRECTION FOR SINUOSITY (1=yes, 0=no) [VALUE, def=1.0]
1 1.5
```

A listing of `1 1.5` tells QTRACER2 to correct the radial distance for sinuosity by a factor of $1.5\times$. However, if no value is listed, a default equal to 1.0 is supplied. The sinuosity factor is limited to a range of $1.0 \leq 3.0$.

### 6.6.9. Flow Medium

QTRACER2 allows the user to decide if the flow system conforms to a subsurface channel such as a typical karst solution-conduit or mine tunnel (*e.g.*, tubular), surface channel such as a small stream or large river (*e.g.*, Missouri River), porous medium (*e.g.*, granular aquifer), or fracture opening (*e.g.*, planar) or set of fractures. If it is a fractured-rock system, 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 occurred via a single fracture. A porosity value has no effect for flow through subsurface channels or surface channels. A porosity value also has no effect on a porous-media flow system in QTRACER2 if a hydraulic conductivity value is missing.

```
FLOW MEDIUM: POROSITY (1=subsurface channel, 2=surface channel,
        3=porous medium, 4=fractured medium) [VALUE, def=1.0]
1
```

For `QTRACER.DAT`, a value of 1 tells QTRACER2 to consider subsurface-channel flow only; a porosity value does not need to be entered because QTRACER2 automatically sets a default value of 1.0.

### 6.6.10. Porous-Media and Fracture Units

If tracer migrated through a porous medium, then the user would list the estimated hydraulic conductivity by first recording a units identifier (*e.g.*, 1) and then an actual value representing the hydraulic conductivity.

Alternatively, if the tracer migrated through a fractured-rock system, then the user would list the fracture(s) measured or estimated height units. Otherwise, QTRACER2 will do its best to estimate the height, although the estimated value may not be very reliable.

```
IF POROUS FLOW: UNITS, HYDR. COND. (1=m/s, 2=m/hr, 3=ft/s, 4=m/hr, 0=null)
IF FRACTURE(S) FLOW: UNITS, HEIGHT (1=m, 2=ft, 0=null) [VALUE]
0 0.0
```

The flag 0 is irrelevant here because flow is a subsurface channel. However, for porous media or fracture flow, the flag 0 tells QTRACER2 that fracture height is unknown and must be estimated by QTRACER2.

### 6.6.11. Output File Name

QTRACER2 requires that an output *filename* be given so that the results may be written to an "output 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
Q1.OUT
```

The output file name Q1.OUT is used here because it allows for easy deletion without inadvertently deleting the original input files. Any filename is allowed by QTRACER2, although the user may not want to use a name that is excessively long.

### 6.6.12. Sample Data Interpolation

QTRACER2 is very good at data interpolation. It relies on a piecewise cubic Hermite to determine the best possible interpolant for the given data.

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

This requestor is asking if the user would like to interpolate the data. A 0 means NO and the user may move on. A 1 (QTRACER.DAT example) means YES and the user then must inform QTRACER2 of the *MINIMUM* number of knot points to be created by the interpolation algorithm.

To create an interpolated data file, 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 QTRACER2 that data interpolation is desired and that $\geq 200$ knots points (interpolated data points) are required. Any value other than `200` could be used as computer 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 is then stored and can be viewed later or deleted as desired.

```
NAME OF THE INTERPOLATED OUTPUT VALUES FILE
Q1.INT
```

The output filename `Q1.INT` is used here because it allows for easy deletion without inadvertently deleting the original input files. Any file name is allowed by QTRACER2, although the user may not want to use a name that is excessively long. If data interpolation is not requested above, this requestor is ignored by QTRACER2.

### 6.6.14. Sample Data Extrapolation

QTRACER2 is also very good at data extrapolation, but it is up to the user to determine the method 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 `QTRACER.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.

QTRACER2 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 the interpolation flag is 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). Any one 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 data points (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 QTRACER.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. on page 61 using the pull-down menus.

Sometimes the curve may look somewhat odd; this occurs because the interpolation algorithm used for smooth plotting sometimes has difficulty jumping to oddly placed data

points[4]. Data interpolation by QTRACER2 will help overcome this effect. Also, fewer than three data points will result in no data smoothing.

More importantly, the shape of the curve drawn through the data points does not necessarily represent the integration. QTRACER2 will perform a much better integration of the curve than appears on the screen, in that it will seamlessly connect the points 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 QTRACER2 is 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.

Using QTRACER2 for automatic PostScript output does *NOT REQUIRE* that the data *filenames* be shorter than six characters. For the initial data file, the new name adds underscores and extensions as appropriate. For example, the Qtracer.dat data file would result in a PostScript plot file named *Qtracer_dat.ps* to identify it as a plot of the actual data file as recorded by the user. Likewise, an interpolated data file would be named *Qtracer_int.ps* and a Chatwin data file would be named *Qtracer_cht.ps*. However, all subsequent PostScript plot data file would conform to user chosen output file names. For example, a normalized tracer mass file would be named *Q1_nrm.ps*.

***Manual Bitmapped Files*** Bitmapped files of all screen plots can be created very easily by QTRACER2. These will usually be done when QTRACER2 is not being run in batch mode. This is accomplished using the **File** pull-down menu described in Section 5.6.1. on page 61

### 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

---

[4]This problem was evident in Version 1.0 of QTRACER mainly due to the bezier algorithm used for data smoothing. Version 2 of QTRACER (QTRACER2) does not exhibit this problem so readily because the bezier algorithm has been replaced by a cubic Hermite algorithm.

was requested by the user.

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

This example `0 1 1 0` tells QTRACER2 to do nothing for the `QTRACER.DAT` data file because no data interpolation was requested. If interpolation data had been requested, then `0 1 1 0` would tell QTRACER2 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, QTRACER2 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 data points with a line. That is, the Chatwin parameters may be examined (`CHECK`), printed to a file (`PRINT`), 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 PRINT PLOT OPLOT)
0 0 1 0
```

The switches, `0 0 1 0` for the `QTRACER.DAT` example, inform QTRACER2 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. QTRACER2 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 creation of a CXTFIT file (`CXTFIT`) and use the original injected tracer mass (`Min`) or the recovered tracer mass (`Mout`) 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 QTRACER2 not to create a CXTFIT2.0 file and not to use

either the mass injected or mass recovered in file creation. If a CXTFIT2.0 file option was set to `1` and the other two options set to `0`, 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 — QTRACER2 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 QTRACER2 was forced to use the method of moments to estimate dispersion, then the "`D`" parameter listed in the CXTFIT2.0 created file could 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 QTRACER2, 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\Q1.ADV
```

The data line, `C:\VANGENU\CXT\Q1.ADV`, tells QTRACER2 to create the CXTFIT2.0 file at the above listed path where the executable version of CXTFIT2.0 is stored. Actually, the requestor is ignored in this instance because QTRACER2 was informed above not to create a CXTFIT2.0 file.

Any of the files that QTRACER2 creates (except as by `OPLOT`) can be given a path for file storage.

### 6.6.19.   Normalized Tracer Concentration

The time-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 BTCs 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 (`1=on, 0=off`).
```
FLAG FOR NORMALIZED CONCENTRATION VALUES FILE (1/0)
1
```

***Name of Normalized Concentration File for Mass*** As with all other files created by QTRACER2, a filename must be provided before QTRACER2 can create the file.
```
NAME OF FILE FOR NORMALIZED CONCENTRATION VALUES (VALID IF FLAG=1)
Q1.NRM
```
A filename 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 QTRACER2 to 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 BTCs 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 (`1=on, 0=off`).
```
FLAG FOR NORMALIZED TRACER LOAD FILE (1/0)
1
```

***Name of Normalized Concentration File for Load*** As with all other files created
by QTRACER2, a filename must be provided before QTRACER2 can create the file.

```
NAME OF FILE FOR NORMALIZED TRACER LOAD VALUES (VALID IF FLAG=1)
Q1.LOD
```

A filename 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 QTRACER2 to 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

$$\frac{(t - \bar{t}\,)}{\sigma_t} \tag{70}$$

and concentration data may be rewritten by

$$\frac{C}{C_p} \tag{71}$$

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.

Breakthrough curves generated by multiple tracer tests conducted from the same
tracer-release point to the same tracer-recovery point conducted under differing hyrdologic
conditions may be examined by plotting each standardized BTC on the same graph. When
comparing the BTCs, it is useful to note the skewness and kurtosis (see Section 3.3.
on page 32) as well as visually noting similarities in the curves of each BTC. Apparent
differences between plotted BTCs, skewness, and/or kurtosis must be critically examined
to determine if the differences may be judged significant.

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***Flag to Create Standardized Data File***   The creation of a standardized dimensionless data file is again performed by the on/off switch described earlier (`1=on, 0=off`).

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

***Name of Standardized Data File***   As with all other files created by QTRACER2, a filename must be provided before QTRACER2 can create the file.

```
NAME OF FILE FOR STANDARDIZED TIME AND CONCENTRATION (VALID IF FLAG=1)
Q1.STN
```

A filename 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 QTRACER2 to display a smooth line on the screen.

### 6.6.22.   Screen Display

QTRACER2 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`. QTRACER2 will pause periodically to allow the user to view the results; RETURN will inform QTRACER2 to continue.

Setting the switch to `0=off` allows QTRACER2 to run in the batch mode. This is 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 computer memory allocation. Because of this problem, QTRACER2 has been programmed to allow for adjustment accordingly by:

1. Using all the time-concentration data, provided computer memory is not exceeded.

2. Averaging blocks of data to create a single data point for each block.

3. Skipping blocks of data.

The more measured data that QTRACER2 can handle the better. Therefore, if QTRACER2 must use less than all the data it will attempt to minimize the size of the blocks it must average or skip.

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

Two sets of data files were created to be "huge" are included on the disk. The first set, `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`, was created from the MULL data set by interpolation and include a "variable" discharge (although discharge did not always vary while being 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 must only be listed if a variable discharge was measured at each sampling interval. For the `QTRACER.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 earlier identified as a variable, then a discharge column must be recorded; if discharge was earlier identified as a constant, 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 is `6` (the second 6 listed).

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 system volumes are to be estimated for a variable discharge, `TIME` must begin with `0.0`. As noted above, zero time is now automatically added when missing from the time-concentration data file.

Conduit volume and Reynolds number can only be calculated if discharge is 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, making calculations for the `RCA.DAT` data sets suspect.

# 7. EXAMPLE ANALYSES FROM QTRACER2

QTRACER2 is very easy and fast to use once the necessary header file and sampling station data files have been created (see Section 6. on page 65). As described in Section 6.2. on page 66, the user need only place the pointer on the QTR icon and *Left Double-Click* to initiate QTRACER2, which introduces the program and prompts for the name of a header file (tracing project file). At this point the user may type any valid header filename (*e.g.*, `Qtracer.D`) or just press `<Enter>` to automatically run the QTRACER2 default file (`Qtracer.D`) and observe proper functioning of QTRACER2.

At this point, QTRACER2 will proceed until finished if the batch mode has been specified (see Section 6.6.22. on page 87). Alternatively, if the user requested screen display, QTRACER2 will pause periodically to allow the user to observe the analytical results as they become available. Simply pressing `<ENTER>` as directed by QTRACER2 will cause QTRACER2 to move to the next available display screen except for the data plot screens. The plot screens require the user to click the *Left Click* anywhere on any particular child window to highlight that window for interactive manipulation using the pull-down menus and for viewing. *Left Clicking* on the **Graphic1** screen returns the user to the data-display screen.

Lastly, if multiple sampling station data files are to be processed by QTRACER2 for a single tracing project file or header file (see Section 6.5. on page 69), then QTRACER2 will enter a loop mode. Upon completion of processing a single sampling station data file, QTRACER2 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, QTRACER2 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. QTRACER.D EXAMPLE OUTPUT

In Section 6.5. on page 69 `QTRACER.D` was used as a sample tracing project file or header file. `QTRACER.D` referenced the sampling station data file, `QTRACER.DAT` (Section 6.6. on page 72, and Table 11), that provided all the information necessary for QTRACER2 processing of the data for that sampling station.

### 7.1.1. QTRACER.DAT Tracer-Breakthrough Curve

Figure 16 depicts the basic tracer-breakthrough curve generated and analyzed by QTRACER2. Note that discharge was measured each time a water sample was collected.

### 7.1.2. QTRACER.DAT Chatwin Plot

Figure 17 depicts the data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER2. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER2 where Y = 747.901 + -95.3754 is of the form y = mx + b and Equations (41) and (42) are: $x_1 = 747.901$ and $x_2 = -95.3754$.

### 7.1.3. QTRACER.DAT Output File

Figure 18 depicts the final analytical output generated by QTRACER2. Besides observing the analytical results, note the end of the output file, which depicts the complete results of the analysis. QTRACER2 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. QTRACER.DAT Normalized Tracer Concentration

Figure 19 depicts the normalized tracer concentration data generated by QTRACER2 according to the method described by Mull *et al.* (1988). Note the concentration units for the y axis.

### 7.1.5. QTRACER.DAT Normalized Tracer Load

Figure 20 depicts the normalized tracer load data generated by QTRACER2 according to the method described by Mull *et al.* (1988). Note the concentration units for the y axis.

### 7.1.6. QTRACER.DAT Standardized Time-Concentration Data

Figure 21 depicts the standardized-time concentration data generated by QTRACER2 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.
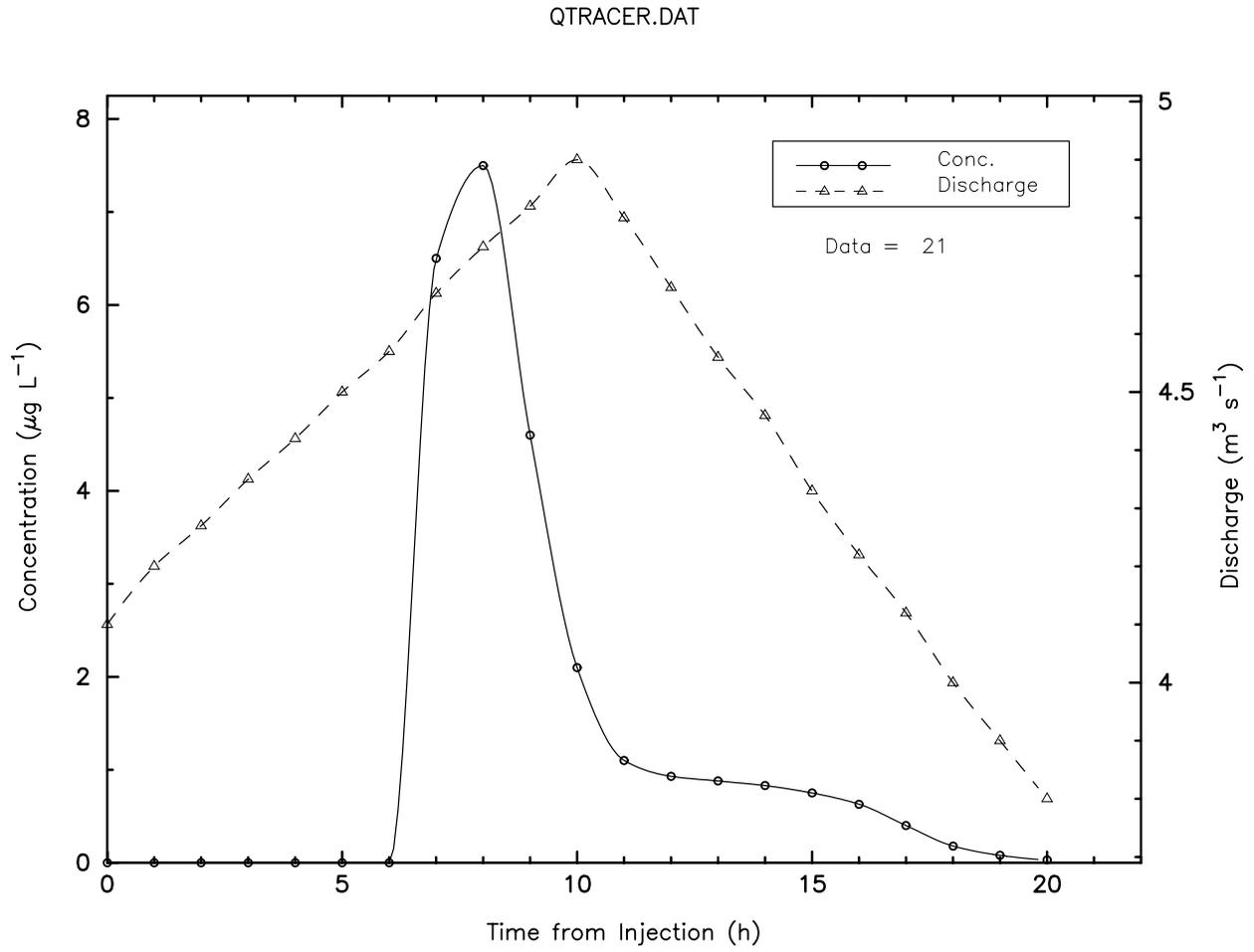
Figure 16. Tracer-breakthrough curve for the `QTRACER.DAT` sampling station data file.
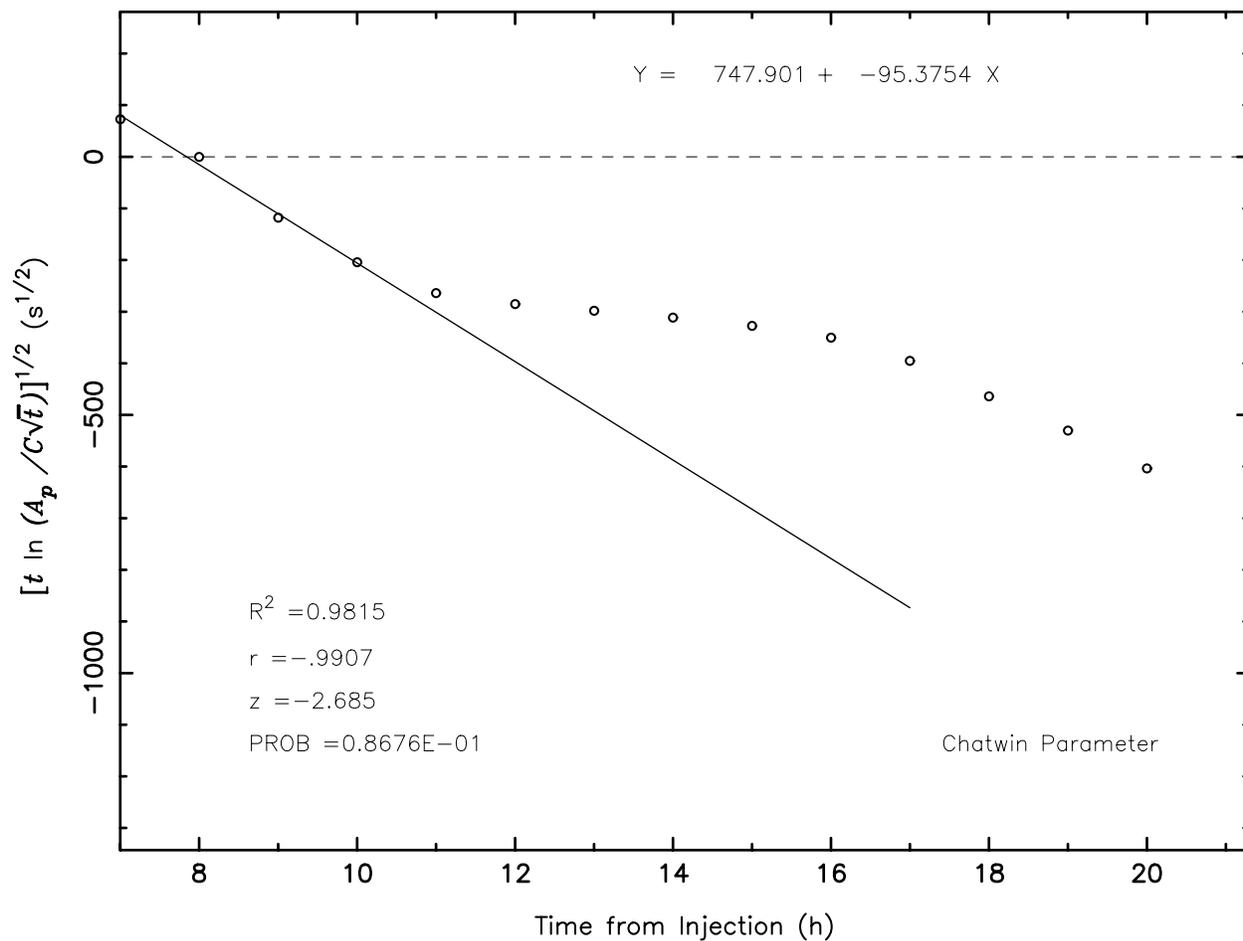
Figure 17. Plot and straight-line fit of the Chatwin parameter for the `QTRACER.DAT` sampling station data file.

```
******************************************************************
*                                                                *
*  Listing of output for:  QTRACER.DAT                           *
*                                                                *
******************************************************************


Limits to integration for the data file:  QTRACER.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 `QTRACER.DAT` sampling station data file.

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```
The mean tracer transit time                           .38629      d
                                                       9.2711      hrs
                                                       556.26      min


Variance for mean tracer time                          .11515E-01  d^2
                                                       6.6325      hrs^2
                                                       23877.      min^2


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



The mean tracer velocity                               6989.5      m/d
                                                       291.23      m/hr
                                                       .80897E-01  m/s


Standard deviation for tracer velocity                 1637.7      m/d
                                                       68.238      m/hr
                                                       .18955E-01  m/s




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


Peclet number                                          67.037
                                                       Advection > Diffusion
```

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

```
The maximum tracer velocity                      9257.1     m/d
                                                 385.71     m/hr
                                                 .10714     m/s


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

Flow-channel cross-sectional area                55.338     m^2

Flow-channel surface area                        .51674E+08  m^2
 Tracer sorption coefficient (channel)           .13016E-04  m

Hydraulic head loss along channel                .12078E-01  m
 Based on a friction factor                      .11254


Viscous-flow sublayer along walls                1.3779     mm

Estimated Reynolds number                        .59564E+06
 Based on an estimated tube diameter             8.3939     m


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

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

Molecular mass transport parameters


  Shear velocity                               .17006E-01  m/s


  Estimated Schmidt number                  1140.0


  Estimated Sherwood number                14926.


  Mass transfer coef. from wall to flow     .17782E-05  m/s


  Molecular diffusion layer thickness      .56238      mm


Percent recovery of tracer injected       99.552      %


Accuracy index (0.0 = Perfect Recov.)      .4481E-02


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

```
*******************************************************************
*                                                                 *
*  Listing of output for:   QTRACER.DAT                           *
*                                                                 *
*******************************************************************


Total quantity of tracer recovered              .44798      kg
                                                447.98       g




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

Total aquifer surface area estimate             .51674E+08  m

Final tracer sorption coefficient               .13016E-04  m



Percent recovery of tracer injected             99.552      %
Accuracy index (0.0 = Perfect Recov.)           .4481E-02
```

Figure 18. Output file for the `QTRACER.DAT` sampling station data file (continued).
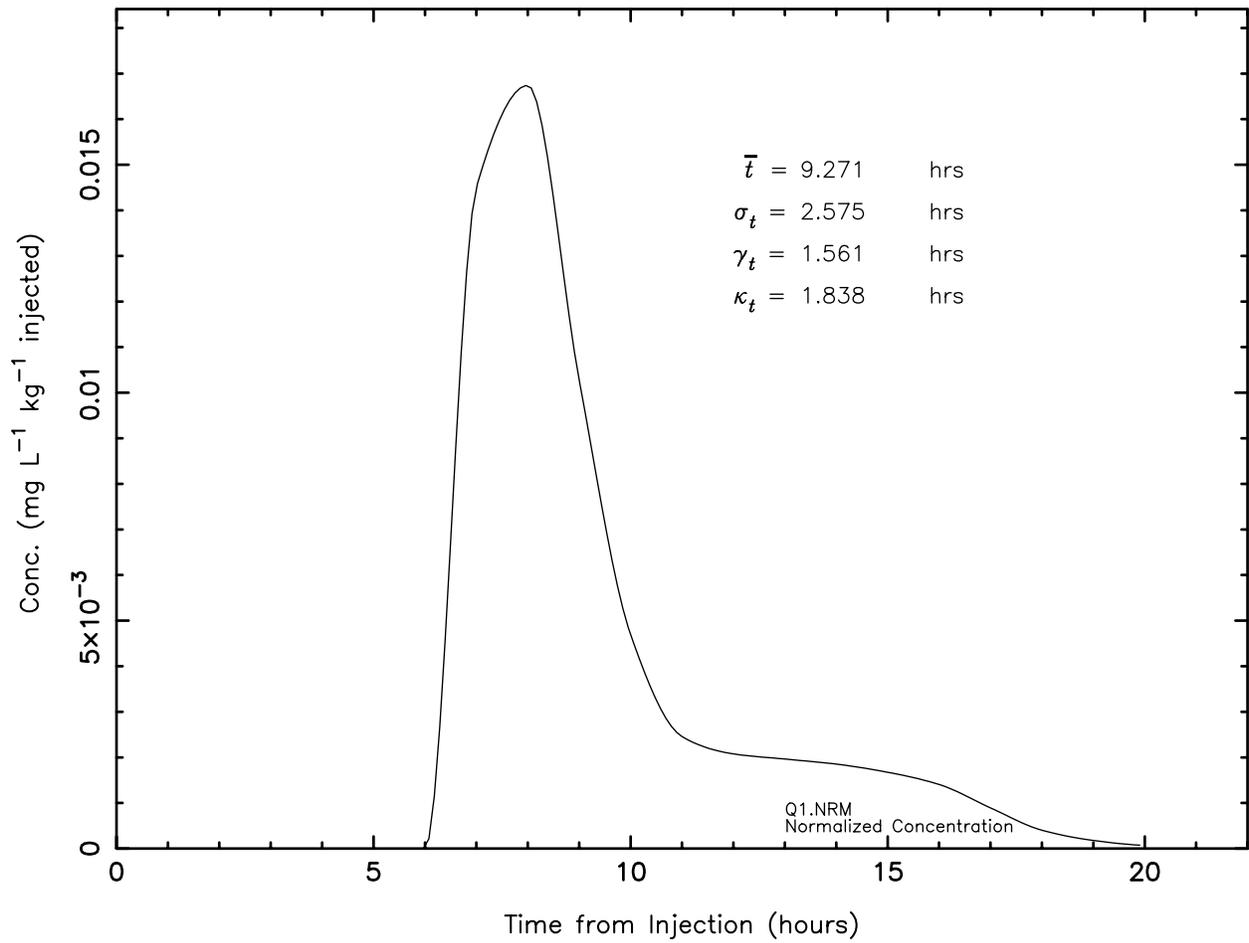
Figure 19. Normalized tracer concentration data for the QTRACER.DAT sampling station data file.

QTRACER.DAT

$\overline{t}$ = 9.271 hrs
$\sigma_t$ = 2.575 hrs
$\gamma_t$ = 1.561 hrs
$\kappa_t$ = 1.838 hrs

Q1.LOD
Normalized Load
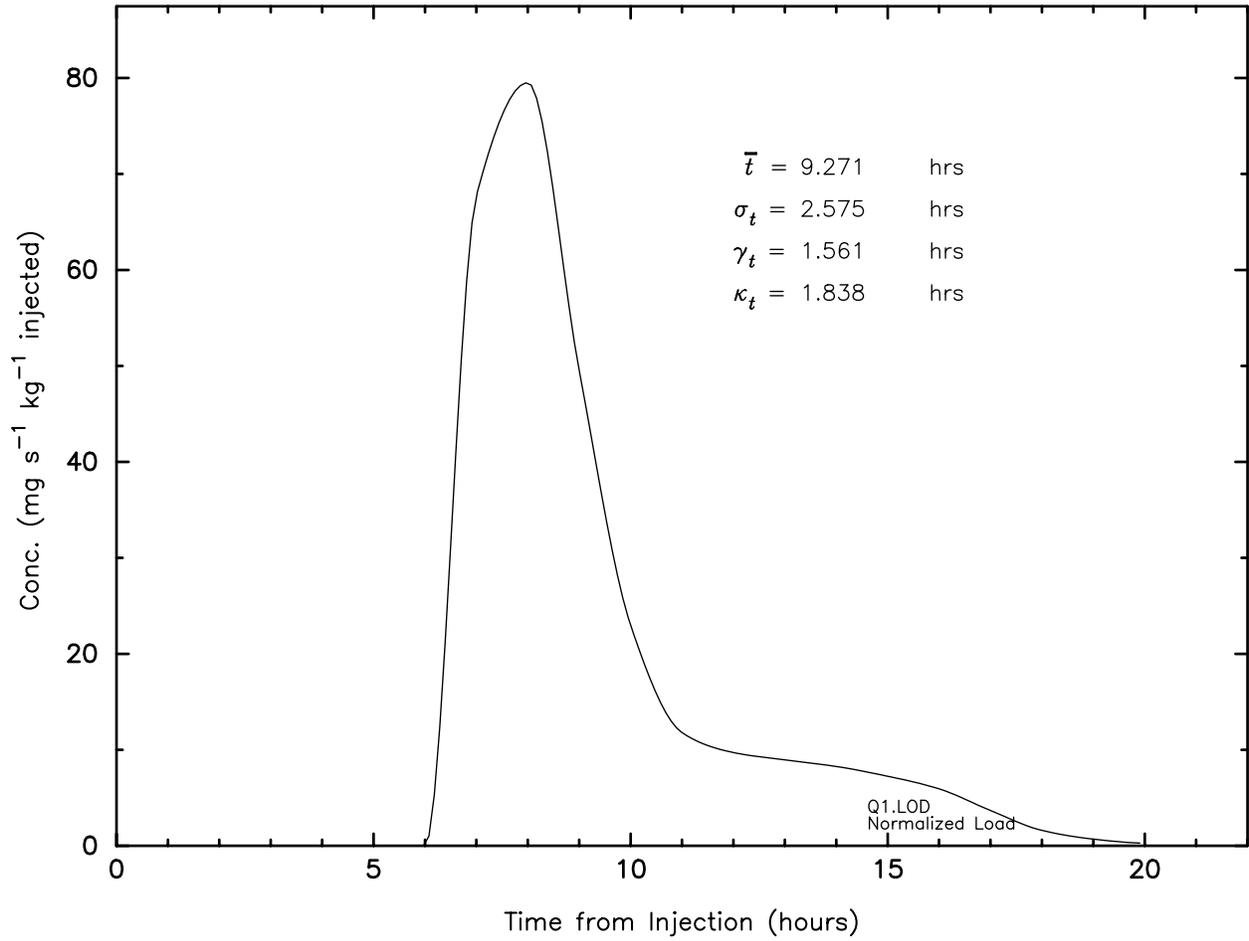
Figure 20. Normalized tracer load data for the QTRACER.DAT sampling station data file.
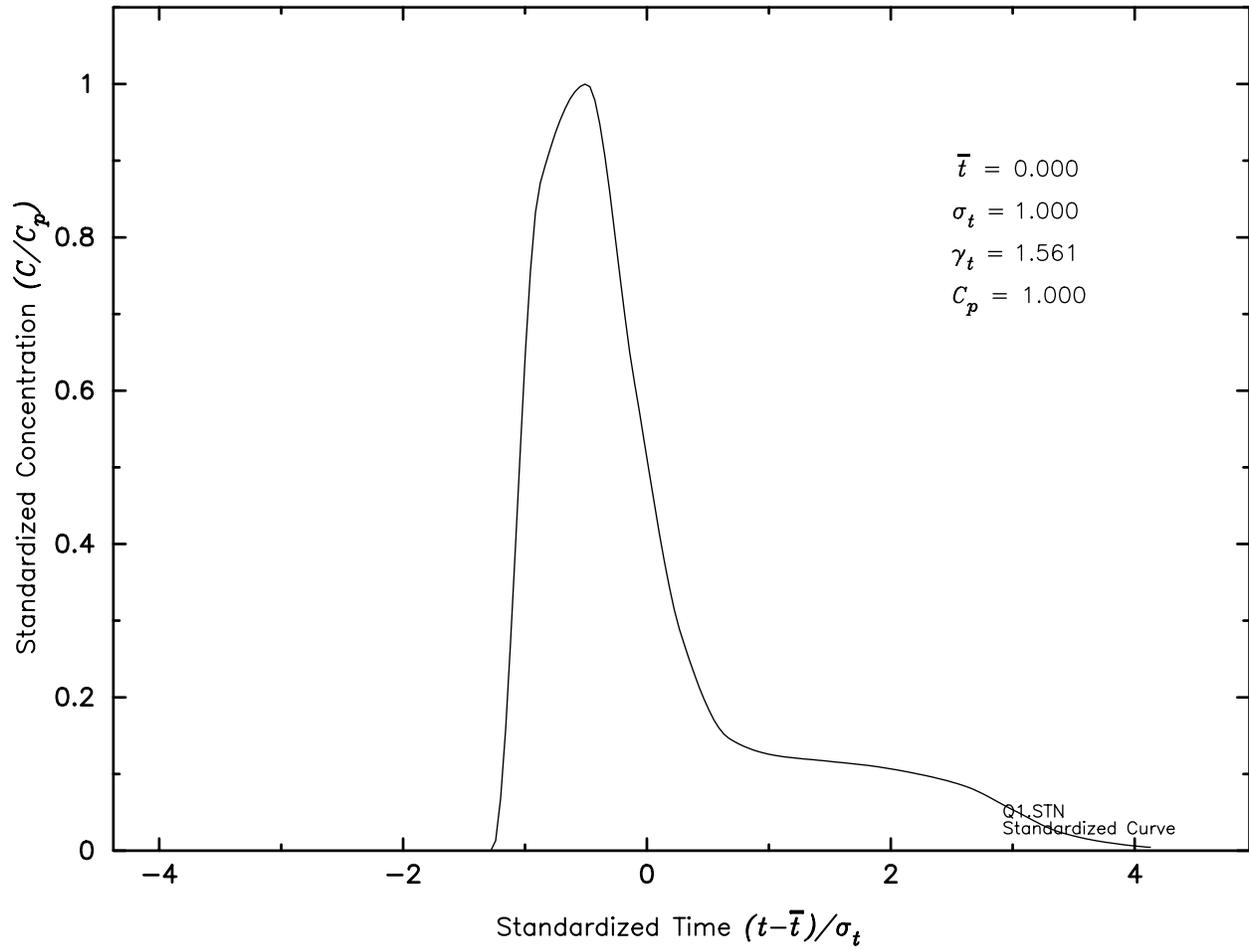
Figure 21. Standardized time-concentration data for the QTRACER.DAT sampling station data file.

## 7.2. RCA.D EXAMPLE OUTPUT

In Section 4.1. on page 50 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 QTRACER2 and references the sampling station data file, `RCA.DAT` (Table 11), that provides all the relevant information necessary for QTRACER2 processing of the data obtained for that sampling station.

### 7.2.1.  RCA.DAT Tracer-Breakthrough Curve

Figure 22 depicts the basic tracer-breakthrough curve generated by QTRACER2 and analyzed by QTRACER2. 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 QTRACER2 and analyzed by QTRACER2. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER2.

### 7.2.3.  RCA.DAT Output File

Figure 24 depicts the final analytical output generated by QTRACER2. Besides observing the analytical results, note the end of the output file, which depicts the complete results of the analysis. QTRACER2 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 QTRACER2 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 QTRACER2 according to the method described by Mull *et al.* (1988). Note the concentration units for the y axis.
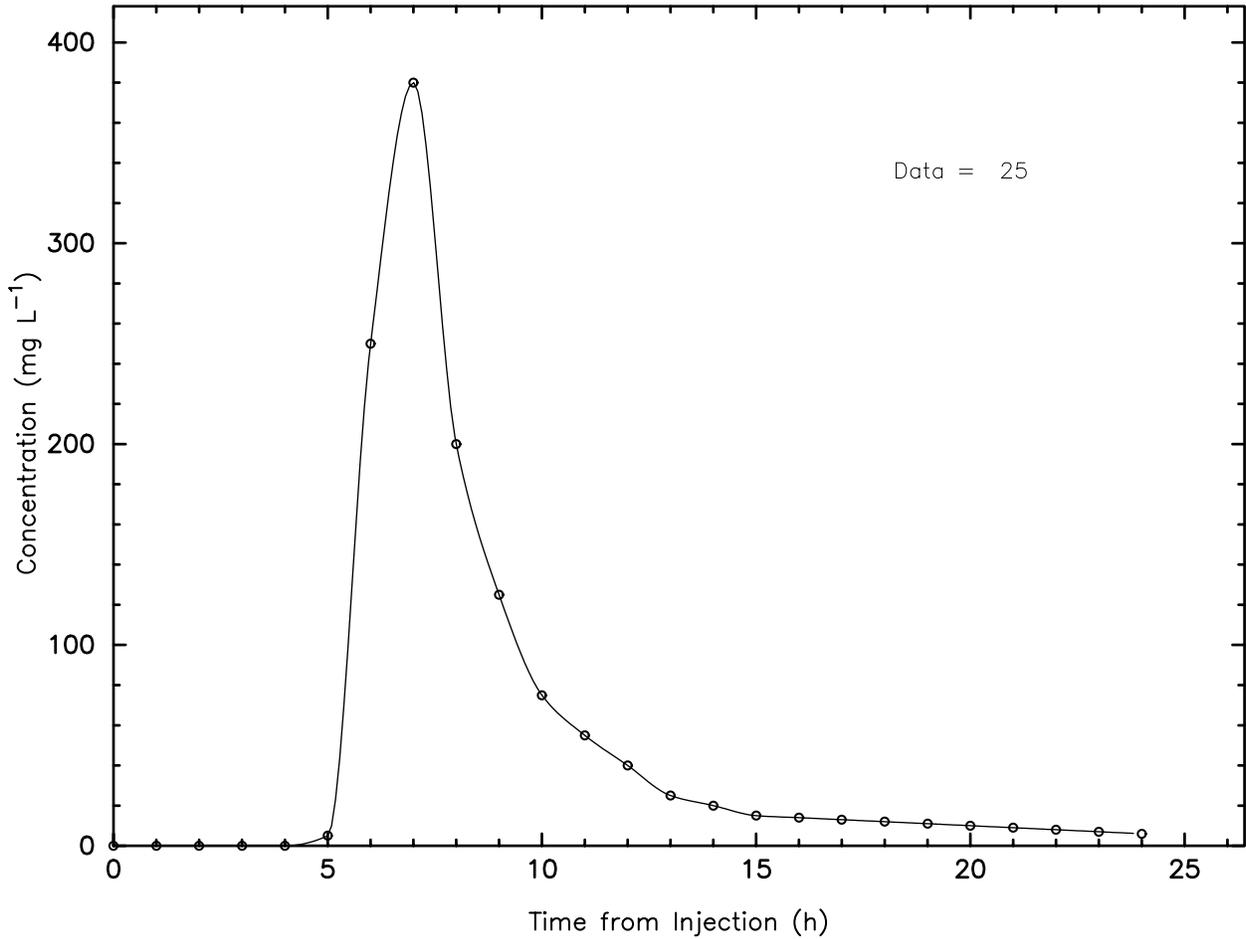
Figure 22. Tracer-breakthrough curve for the RCA.DAT sampling station data file.

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               33.528      m
                                                  (110.00       ft)
Uncorrected for sinuosity



Time to leading edge (first arrival)               5.0000      hrs



Time to peak tracer concentration                  6.9999      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                            .35853      d
                                                        8.6048      hrs
                                                        516.24      min


Variance for mean tracer time                           .21200E-01  d^2
                                                        12.211      hrs^2
                                                        43961.      min^2


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



The mean tracer velocity                                93.753      m/d
                                                        3.9064      m/hr
                                                        .11111E-02  m/s


Standard deviation for tracer velocity                  29.204      m/d
                                                        1.2168      m/hr
                                                        .33801E-03  m/s




Dispersion coefficient                                  .31943E-03  m^2/s
Longitudinal dispersivity                               .29437      m


Peclet number                                           113.90
                                                        Advection > Diffusion
```

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

```
The maximum tracer velocity                        160.94     m/d
                                                   6.7057     m/hr
                                                   .18627E-02 m/s


Flow-channel volume estimate                       11.726     m^3

Flow-channel cross-sectional area                  .34974     m^2

Flow-channel surface area                          21237.     m^2
 Tracer sorption coefficient (channel)             .83208E-01 m

Hydraulic head loss along channel                  .30391E-06 m
 Based on a friction factor                        .10076E-01


Estimated Reynolds number                          635.17
 Based on an estimated tube diameter               .66731     m

 and an hydraulic conductivity                     .11971E+06 m/s


Estimated Froude number                            .47862E-03
 Based on an estimated hydraulic depth             .52411     m
```

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

```
Molecular mass transport parameters


   Shear velocity                              .21585E-03  m/s


   Estimated Schmidt number                    1140.0


   Estimated Sherwood number                   139.57


   Mass transfer coef. from wall to flow       .20915E-06  m/s


   Molecular diffusion layer thickness         4.7813      mm


Percent recovery of tracer injected           .65922      %


Accuracy index (0.0 = Perfect Recov.)         .9934
```

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

```
**********************************************************************
*                                                                    *
*  Listing of output for:  RCA.DAT                                   *
*                                                                    *
**********************************************************************


Total quantity of tracer recovered              1.7403     kg
                                                1740.3     g




Total aquifer volume estimate                   11.726     m^3

Total aquifer surface area estimate             21237.     m

Final tracer sorption coefficient               .83208E-01 m



Percent recovery of tracer injected             .65922     %
Accuracy index (0.0 = Perfect Recov.)           .9934
```

Figure 24. Output file for the `RCA.DAT` sampling station data file (continued).
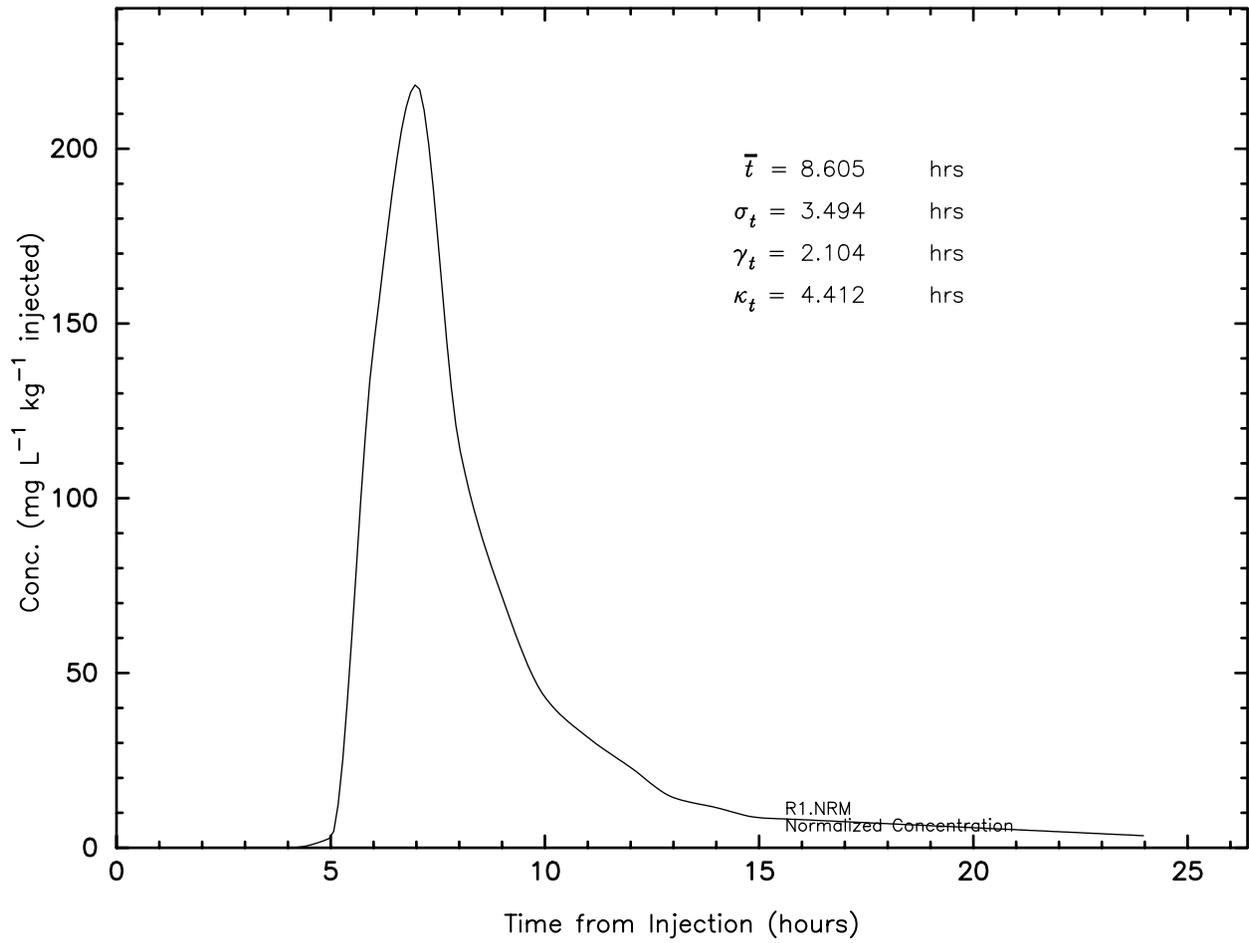
Figure 25. Normalized tracer concentration data for the `RCA.DAT` sampling station data file.

$\overline{t}$ = 8.605    hrs

$\sigma_t$ = 3.494    hrs

$\gamma_t$ = 2.104    hrs

$\kappa_t$ = 4.412    hrs

R1.LOD
Normalized Load

Conc. (mg s$^{-1}$ kg$^{-1}$ injected)

Time from Injection (hours)
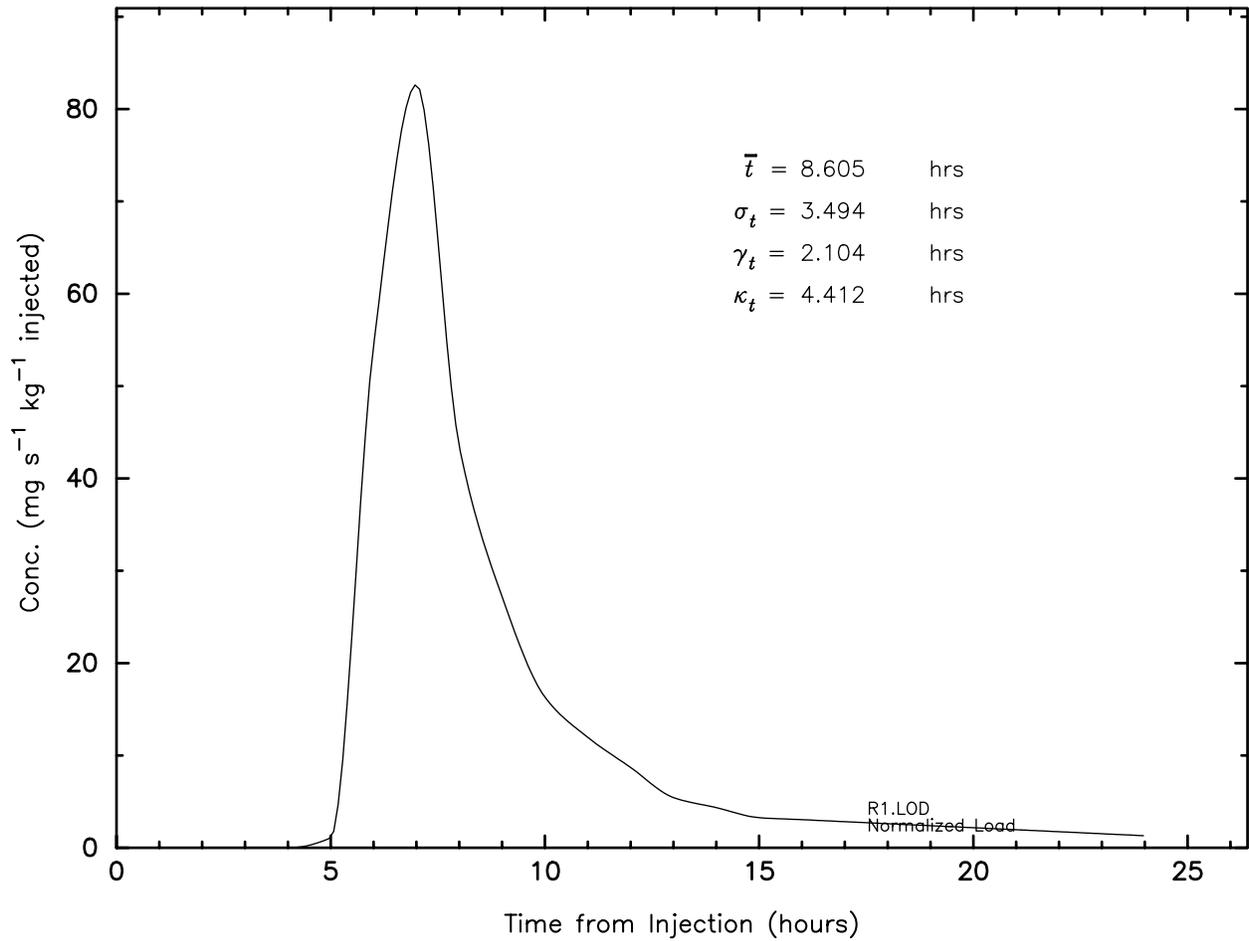
Figure 26. Normalized tracer load data for the `RCA.DAT` sampling station data file.

111

### 7.2.6. RCA.DAT Standardized Time-Concentration Data

Figure 27 depicts the standardized-time concentration data generated by QTRACER2 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.

### 7.3. ANALYSIS ASSESSMENT OF THE QTRACER AND RCA EXAMPLE DATA FILES

From the two examples (QTRACER and RCA), it is apparent that QTRACER2 is not affected by variable discharges versus a constant discharge. QTRACER2 is also not affected by recovery at a spring versus recovery at a monitoring well.

The QTRACER data set resulted in nearly perfect mass recovery. Had the QTRACER data set been analyzed according to the description given in Section 4. on page 48, the user would have noted a mass recovery $> 100\%$. The efficient integration algorithms used by QTRACER2 results in a more reliable mass balance.

QTRACER2 results for the RCA data set were quite similar to those presented in Section 4.1.1. on page 51 QTRACER2 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 $\delta_m$ 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 $\delta_m$ may be achieved from (Dreybrodt, 1988, p. 172)

$$N_{sh} = D_C/\delta_m \tag{72}$$

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

$$N_{sh} = 0.023 N_R^{0.83} N_{sc}^{1/3} \tag{73}$$

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

$$N_{sh} = 3.65 + \frac{0.668(D_C/x_s)N_R N_{sc}}{1 + 0.04[(D_C/x_s)N_R N_{sc}]^{0.67}} \tag{74}$$

RCA.DAT
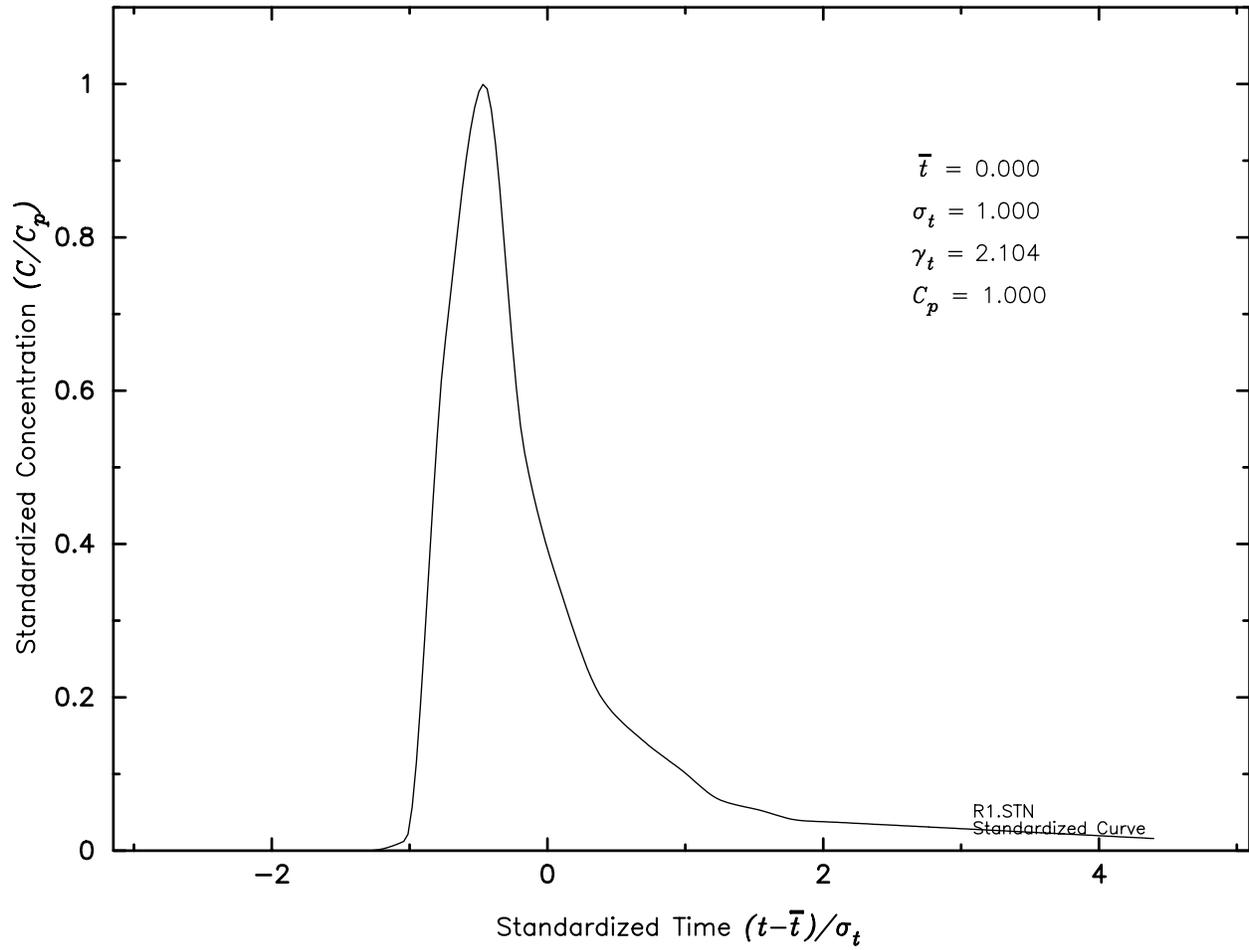


Figure 27. Standardized time-concentration data for the RCA.DAT sampling station data file.

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

$$N_{sh} = \frac{k_f D_C}{D_m} \tag{75}$$

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

$$N_{sc} = \frac{\mu}{\rho D_m} \tag{76}$$

It will be noted here that $D_m = 1.0 \times 10^{-9}$ (L$^2$ T$^{-1}$) is taken as a general value for all tracer tests in QTRACER2 because it is too demanding that every possible tracer diffusion coefficient be identified in QTRACER2. It is also assumed that the average user of QTRACER2 will be unfamiliar with the appropriate value for $D_m$, making it impractical to expect a user to provide an accurate value. For these reasons, any calculations using $D_m$ should be regarded as being only rough approximations.

# 8.   QTRACER ANALYSIS OF OTHER HYDROLOGICAL SETTINGS

The previous version of QTRACER2 (QTRACER) was primarily designed for analysis of BTCs from tracing tests conducted in karstic terranes (*e.g.*, solution conduits) and fractured-rock terranes.   The previous version noted that BTCs conducted in other hydrological systems could be analyzed as well, but that much of the latter results may not be relevant (*e.g.*, Froude number for a porous-media tracer test) and the user had to know which parameters to ignore. However, as explained in Section 6.6. on page 72 (see also Figure 15 on page 73) a new sampling station data file entry addressing the type of hydrological system is provided for in QTRACER2.

## 8.1.   SURFACE-WATER AND POROUS-MEDIA EXAMPLES

QTRACER2 now allows an entry for the type "FLOW MEDIUM" with an additional entry for the "POROSITY":

**Subsurface Channel = 1** A subsurface channel is considered representative of any type of karstic-solution conduit, mine shaft or tunnel, or any other type of submerged conduit.

**Surface Channel = 2** A surface channel is considered representative of any surface-water flow from a very small creek to a large river.

**Porous Medium = 3** Porous medium is exactly what it sounds like; any type of flow through porous media.  This can be a granular aquifer (*e.g.*, alluvial aquifer) that flows through a packed column in the laboratory. If porous-media flow is chosen, then the user has the option of including a porosity value and a hydraulic conductivity value.

**Fractured Medium = 4** This last item addresses flow through a fractured-rock aquifer in which a fracture porosity is important or flow through a single linear fracture (porosity = 100%). If fracture flow is chosen, the user has the option of including an estimated porosity value and an estimated fracture height value.

### 8.1.1.   Surface-Water Example

A small stream, Uvas Creek, was traced in 1976 using a steady three hour injection of 1068 g of Cl− in late summer during a low-flow period (Bencala and Walters, 1983; Zand, *et al.*,

1976). The emphasis of the tracing test was to investigate the mass-transport processes in a small stream. The experimental study was limited to a 610 m reach with widths ranging from 0.3 to 4 m. Flow rate at the time of the study was 45.0 m$^3$ h$^{-1}$. Time-concentration measurements were taken at selected reaches where measured flow rates varied slightly from 45.0 m$^3$ h$^{-1}$. For this evaluation, tracer recovery at reach 281 m was used. The channel was composed of a rough bed with alternating pools and riffles and a steep slope (0.03 m m$^{-1}$).

This study included several sampling stations along the entire reach of the study. In this particular case, individual runs for each sampling station should be run by QTRACER2 because summation function built into QTRACER2 would incorrectly sum the results for the same tracer-recovery data.

Figure 28 and Figure 29 are the BTC and Chatwin plots of the UVAS Creek data set, respectively. Figure 30 is the output file generated by QTRACER2 on the Uvas Creek data set.

A cursory inspection of Figure 28 will show that plotting was initiated at some value greater than zero. Background Cl$^-$ concentrations at the site were taken as 3.71 mg L$^{-1}$ and are included in the data file for plotting. The background concentration is subtracted from the actual data file prior to any actual data analysis.

It will be noted that Figure 30 differs in some unique ways from Figures 18 and 24 (pages 94 and 105, respectively). For example, both Figures 18 and 24 provide an estimate for the standard deviation for the mean tracer velocity, but no such listing is provided in Figure 30. No standard deviation for mean tracer velocity could be estimated for the UVAS281.DAT data set because the pulse-injection time exceeded the mean time of travel. As indicated in Section 3.3.1. on page 32, this calculation is not trivial. More significant is the fact that the upper limit to integration was necessarily changed from 29.867 hours to 4.3333 hrs (Figure 30) because tracer release was of a long-pulse type.

Transport-parameter estimates by QTRACER2 appears to be excellent. For example, QTRACER2 estimated flow velocity to be 0.038 m s$^{-1}$ which compares exceptionally well with the published velocity of 0.037 m s$^{-1}$ (Zand *et al.*, 1976; Bencala and Walters, 1983) obtained from $Q/A$. From Section 3.3.2. (page 36) it will be noted that in general, the Chatwin method should provide a reasonable estimate for longitudinal dispersion even though it is an incorrect method for pulse and continuous releases. Interestingly, by using the Chatwin method, QTRACER2 estimated longitudinal dispersion to be 0.15 m s$^{-1}$ which compares favorably with the published longitudinal dispersion values of 0.24 m$^2$ s$^{-1}$ (Bencala and Walters, 1983) and 0.25 m$^2$ s$^{-1}$ (Zand *et al.*, 1976).
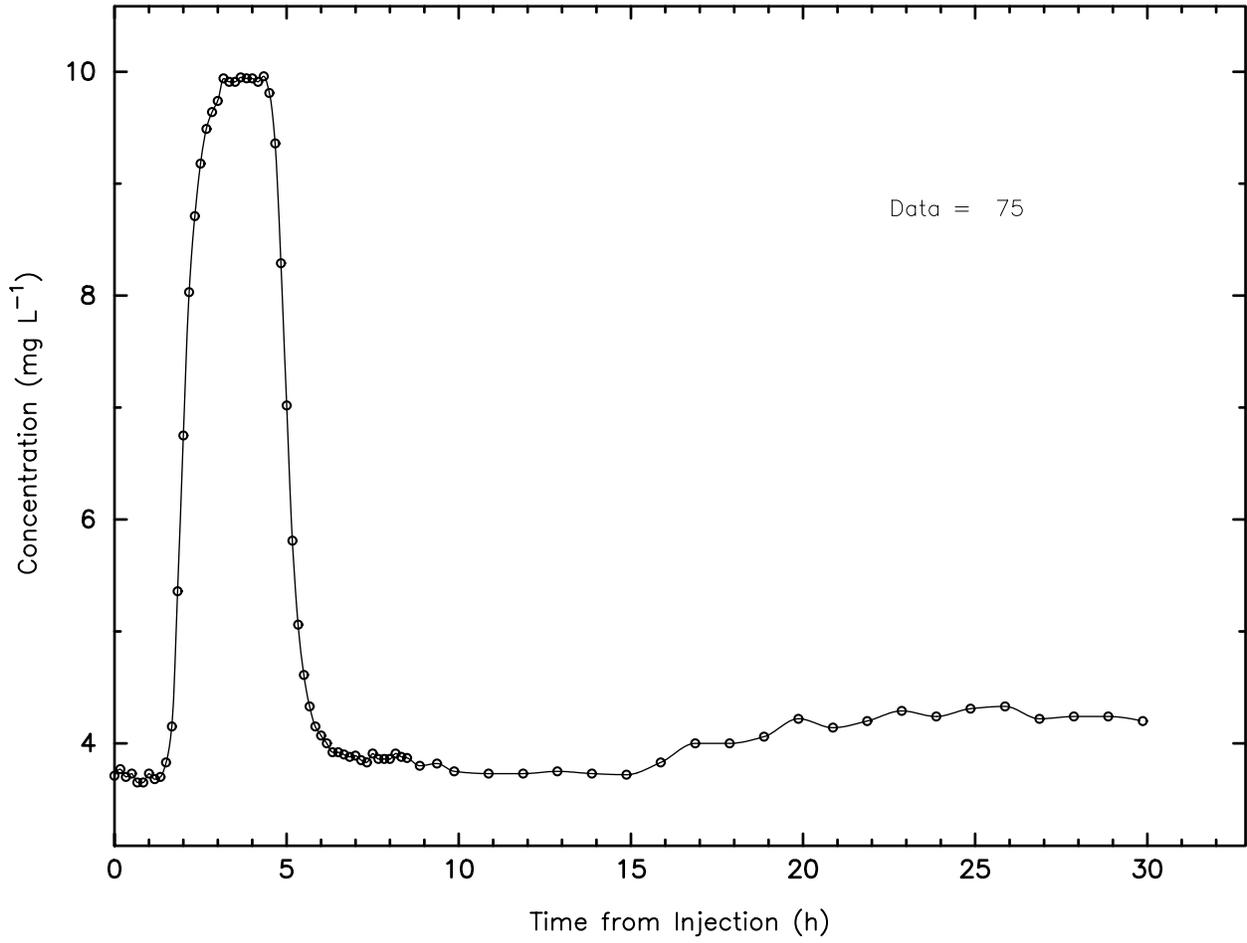
Figure 28. Tracer-breakthrough curve for the UVAS281.DAT sampling station data file.

$$Y = 362.002 + -136.888\ X$$

$[t \ln (A_p / C\sqrt{t})]^{1/2}$ (s$^{1/2}$)

Time from Injection (h)

$R^2 = 0.9913$

$r = -.9956$

$z = -3.062$

PROB $= 0.4368E-02$
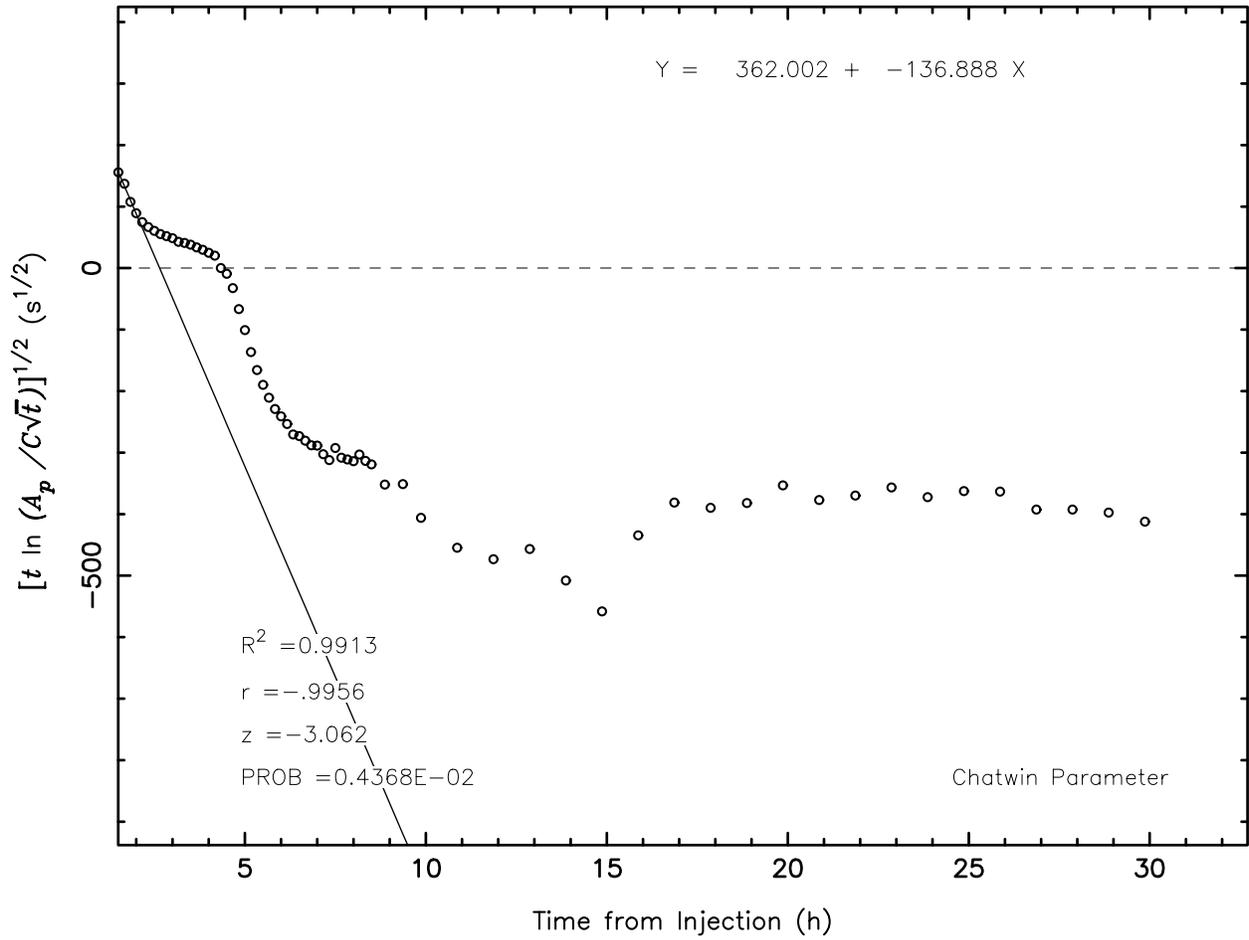
Chatwin Parameter

Figure 29. Plot and straight-line fit of the Chatwin parameter for the `UVAS281.DAT` sampling station data file.

```
**********************************************************************
*                                                                    *
*   Listing of output for:   UVAS281.DAT                             *
*                                                                    *
**********************************************************************


Limits to integration for the data file:   UVAS281.DAT


  Lower integration limit                        .00000      hrs
  Upper integration limit                        29.867      hrs



The quantity of tracer recovered                 1.3191      kg
                                                 1391.1       g
                                                 .13191E+07  mg
                                                 .13191E+10  ug



Distance from input to outflow point             281.00      m
Uncorrected for sinuosity



Time to leading edge (first arrival)             .16667      hrs



Time to peak tracer concentration                4.3333      hrs
For a peak tracer concentration                  6.2500      mg/L
```

Figure 30. Output file for the `UVAS281.DAT` sampling station data file.

```
Upper Limit to integration necessarily changed!

 Lower integration limit                          .00000      hrs
 Upper integration limit                          4.3333      hrs



The mean tracer transit time                      .86625E-01  d
                                                  2.0790      hrs
                                                  124.74      min

Variance for mean tracer time                     .27233E-03  d^2
                                                  .15686      hrs^2
                                                  564.71      min^2

Standard deviation for tracer time                .16502E-01  d
                                                  .39606      hrs
                                                  23.764      min



The mean tracer velocity                          3243.9      m/d
                                                  135.16      m/hr
                                                  .37545E-01  m/s



Dispersion coefficient                            .15064      m^2/s
Longitudinal dispersivity                         4.0122      m


Peclet number                                     70.037
                                                  Advection > Diffusion
```

Figure 30. Output file for the UVAS281.DAT sampling station data file (continued).

```
The maximum tracer velocity                          40464.      m/d
                                                     1686.0      m/hr
                                                     .46833      m/s


Flow-channel volume estimate                         104.78      m^3

Flow-channel cross-sectional area                    .37289      m^2

Flow-channel surface area                            .75270E+06  m^2
 Tracer sorption coefficient (channel)               0.0000      m

Hydraulic head loss along channel                    .44516E-01  m
 Based on a friction factor                          1.5189


Viscous-flow sublayer along walls                    .80813      mm

Estimated Reynolds number                            22692.

 Based on an estimated tube diameter                 .68904      m


Estimated Froude number                              .16297E-01
 Based on an estimated hydraulic depth               .54117      m
```

Figure 30. Output file for the `UVAS281.DAT` sampling station data file (continued).

Molecular mass transport parameters

Shear velocity                                        ..28996E-01  m/s

Estimated Schmidt number                              1140.0

Estimated Sherwood number                             991.01

Mass transfer coef. from wall to flow                 .14383E-05  m/s

Molecular diffusion layer thickness                   .69529        mm

Percent recovery of tracer injected                   123.51        %

Accuracy index (0.0 = Perfect Recov.)                 -.2351

```
        ************************************************************************
        *                                                                      *
        *       AN IMPOSSIBLE CONDITION EXISTS! CHECK YOUR UNITS FOR           *
        *       CORRECTNESS OR CHECK TO SEE IF SAMPLE CONTAMINATION            *
        *       HAS OCCURRED (i.e., HAS SOMEONE ELSE BEEN INJECTING            *
        *       THE SAME TRACER MATERIAL IN THE AREA?).  ALSO CHECK            *
        *       YOUR LIMITS TO INTEGRATION AND YOUR DISCHARGE ESTIMATES.       *
        *       DISCHARGE ESTIMATION ERRORS ARE VERY COMMON. TRACER           *
        *       RECOVERY SHOULD NOT BE GREATER THAN 100% AND THE              *
        *       ACCURACY INDEX SHOULD NOT BE LESS THAN ZERO.                  *
        *                                                                      *
        ************************************************************************
```

Figure 30. Output file for the UVAS281.DAT sampling station data file (continued).

```
    *******************************************************************
    *                                                                 *
    *  Listing of output for:  UVAS281.DAT                            *
    *                                                                 *
    *******************************************************************


Total quantity of tracer recovered                    1.3191      kg
                                                       1391.1      g




Total aquifer volume estimate                         104.78      m^3

Total aquifer surface area estimate                   .75270E+06  m

Final tracer sorption coefficient                     0.0000      m


Percent recovery of tracer injected                   123.51      %
Accuracy index (0.0 = Perfect Recov.)                 -.2351



        ********************************************************************
        *                                                                  *
        *       AN IMPOSSIBLE CONDITION EXISTS! CHECK YOUR UNITS FOR        *
        *       CORRECTNESS OR CHECK TO SEE IF SAMPLE CONTAMINATION         *
        *       HAS OCCURRED (i.e., HAS SOMEONE ELSE BEEN INJECTING         *
        *       THE SAME TRACER MATERIAL IN THE AREA?).  ALSO CHECK         *
        *       YOUR LIMITS TO INTEGRATION AND YOUR DISCHARGE ESTIMATES.    *
        *       DISCHARGE ESTIMATION ERRORS ARE VERY COMMON. TRACER         *
        *       RECOVERY SHOULD NOT BE GREATER THAN 100% AND THE            *
        *       ACCURACY INDEX SHOULD NOT BE LESS THAN ZERO.                *
        *                                                                  *
        ********************************************************************
```

Figure 30. Output file for the `UVAS281.DAT` sampling station data file (continued).

Even more significant in Figure 30 is an error message that appears twice. This error message indicates that more tracer mass was recovered than was injected. Although it appears twice in Figure 30, it only appears in the case when > 100% tracer-mass is recovered. In the case of Figure 30, excess tracer-mass recovery occurred at the single sampling station that was considered. It is possible that individual sampling stations may result in < 100%, but that their sum could result in > 100%.

## 8.1.2.  Porous-Media Example

An injection-withdrawal two-well tracer test consists of injecting water containing tracer into an injection well and withdrawing water from an extraction well at an equal rate so that equilibrium may be established. Such a test was conducted in a soil borrow area at the Barry Steam Plant of the Alabama Power company near Mobile, Alabama in the late summer of 1984. The surface is composed of Quaternary age low-terrace deposits consisting of interbedded sands and clays down to a depth of 61 m. Below these deposits a Miocene series of undifferentiated sands, silty clays, and thin-bedded limestones extend to a depth of 305 m (Molz, *et al.* 1986a, p. 38).

At the Mobile site, bromide was injected into a well over a period of 3.19 days. The entire tracer test lasted 32.5 days (Molz, *et al.* 1986b). The injection and withdrawal wells, separated by a distance of 38.3 m, were operated continuously at 57 m$^3$ h$^{-1}$ (Molz, *et al.* 1986a, p. 55) to cause steady-state conditions between the injection-withdrawal wells. Details of the test are described in (Molz, *et al.* 1986a, p. 52–60, 71) and (Molz, *et al.* 1986b).

Figure 31 and Figure 32 are the BTC and Chatwin plots of the UVAS Creek data set, respectively. Figure 33 is the output file generated by QTRACER2 on the Uvas Creek data set.

As with Figure 30, Figure 33 also differs in some unique ways from Figures 18 and 24 (pages 94 and 105, respectively). For example, both Figures 18 and 24 provide an estimate for the surface area and sorption coefficient, but no such listing is provided in Figure 33. No surface area or sorption coefficient could be estimated for the `MOBILE.DAT` data set because the porous-media systems require some knowledge regarding particle diameter that is not provided for in QTRACER2. In addition, a Froude number is not estimated because a Froude number is not relevant to porous-media systems.
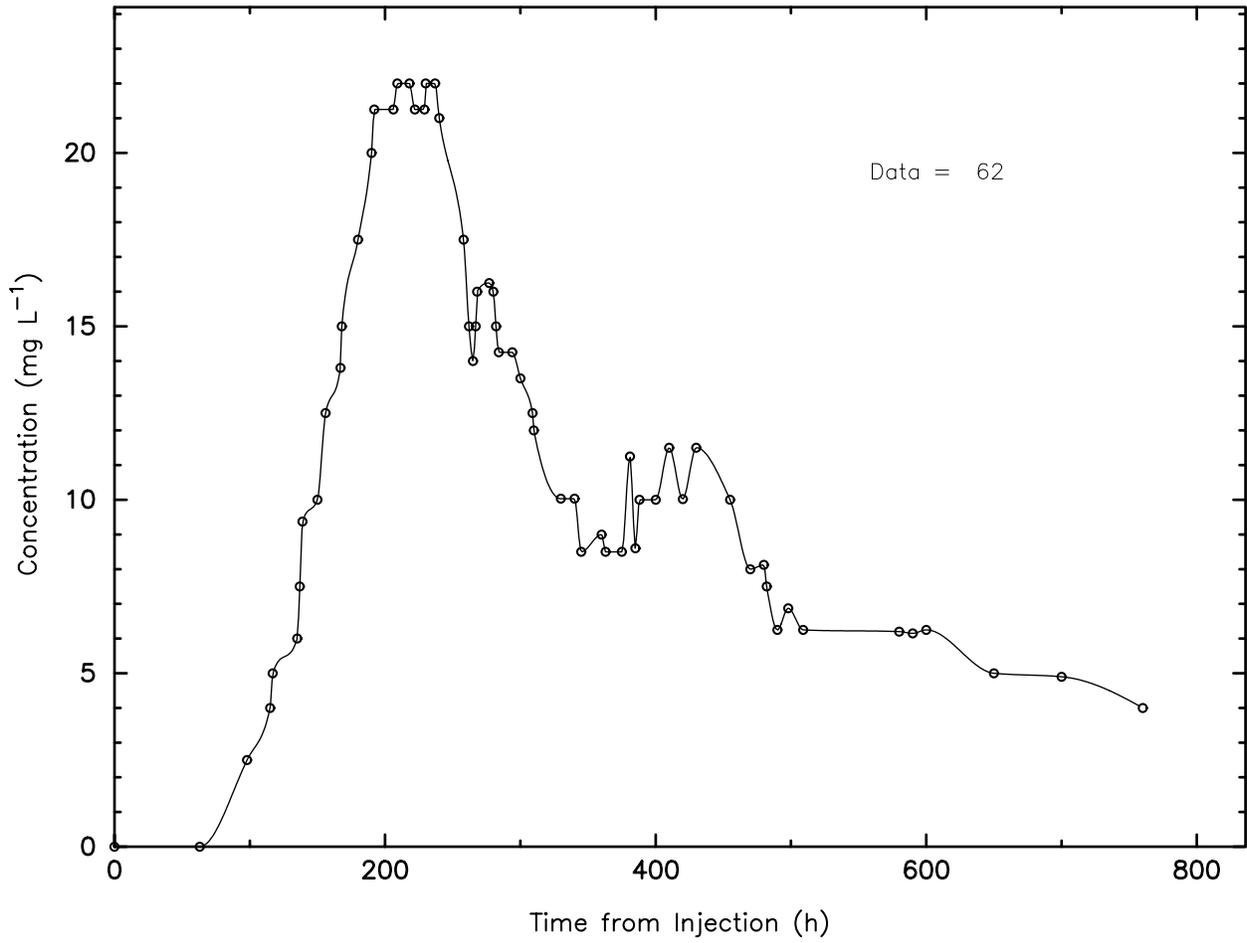
Figure 31. Tracer-breakthrough curve for the `MOBILE.DAT` sampling station data file.

125
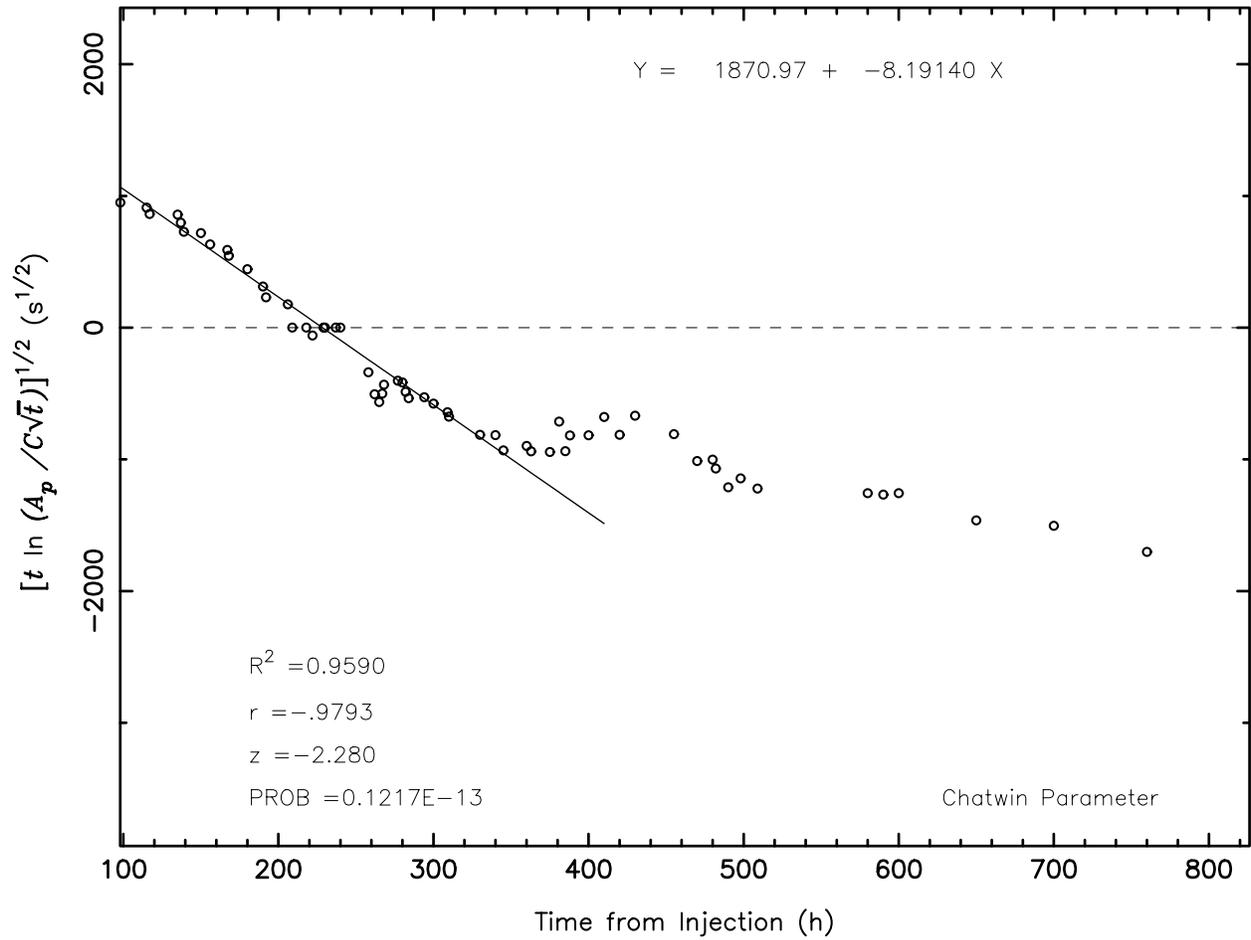
Figure 32. Plot and straight-line fit of the Chatwin parameter for the `MOBILE.DAT` sampling station data file.

```
**********************************************************************
*                                                                    *
*  Listing of output for:   MOBILE.DAT                               *
*                                                                    *
**********************************************************************


Limits to integration for the data file:   MOBILE.DAT


 Lower integration limit                            .00000     hrs
 Upper integration limit                            760.00     hrs



The quantity of tracer recovered                    362.29     kg
                                                   .36229E+06  g
                                                   .36229E+09  mg
                                                   .36229E+12  ug



Distance from input to outflow point                38.300     m
Uncorrected for sinuosity



Time to leading edge (first arrival)                9.8000     hrs



Time to peak tracer concentration                   209.00     hrs
For a peak tracer concentration                     22.000     mg/L
```

Figure 33. Output file for the MOBILE.DAT sampling station data file.

```
The mean tracer transit time                    14.985     d
                                                359.64     hrs
                                                21579.     min


Variance for mean tracer time                   50.094     d^2
                                                28854.     hrs^2
                                                .10387E+09 min^2


Standard deviation for tracer time              7.0777     d
                                                169.86     hrs
                                                10192.     min



The mean tracer velocity                        2.9720     m/d
                                                .12383     m/hr
                                                .34398E-04 m/s


Standard deviation for tracer velocity          2.6669     m/d
                                                .11112     m/hr
                                                .30867E-04 m/s




Dispersion coefficient                          .10476E-03 m^2/s
Longitudinal dispersivity                       3.0456     m


Peclet number                                   12.576
                                                Advection > Diffusion
```

Figure 33. Output file for the `MOBILE.DAT` sampling station data file (continued).

```
The maximum tracer velocity                    9.3796      m/d
                                               .39082      m/hr
                                               .10856E-03  m/s


Transport-zone volume estimate                 20456.      m^3

Transport zone cross-sectional area            534.11      m^2

Hydraulic head loss along channel              .26349E-04  m


Estimated Reynolds number                      .72743E-01
```

Figure 33. Output file for the `MOBILE.DAT` sampling station data file (continued).

```
Molecular mass transport parameters


 Estimated Schmidt number                             1140.0


 Estimated Sherwood number                            1.8708


Percent recovery of tracer injected                  46.388 %


Accuracy index (0.0 = Perfect Recov.)                0.5361
```

Figure 33. Output file for the MOBILE.DAT sampling station data file (continued).

```
*******************************************************************
*                                                                 *
*  Listing of output for:  MOBILE.DAT                             *
*                                                                 *
*******************************************************************


Total quantity of tracer recovered              362.29      kg
                                                .36229E+06  g




Total aquifer volume estimate                   20456.      m^3




Percent recovery of tracer injected             46.388      %
Accuracy index (0.0 = Perfect Recov.)           0.5361
```

Figure 33. Output file for the MOBILE.DAT sampling station data file (continued).

# 9.  DATA INTERPOLATION AND EXTRAPOLATION EFFECTS

As explained in Section 5.1. on page 58, QTRACER2 uses a very efficient data interpolation routine. The primary use of the data interpolation routine is when the user believes that missing data points can be reasonably approximated by data interpolation. For example, if the user believes that unaltered BTCs suggest that data aliasing may have occurred, then data interpolation may be able to confirm or deny if aliasing has actually occurred.

## 9.1.  COMPARISON OF QTRACER.DAT OUTPUT FILES

To illustrate the effect of data interpolation, data extrapolation, and the combined effect of both on a data set exhibiting good mass recovery, the `QTRACER.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.

### 9.1.1.  Interpolated QTRACER.DAT BTC

Figure 34 depicts the interpolated BTC generated and analyzed by QTRACER2. Note that discharge has an interpolated value for each time an interpolated tracer concentration value was created.

### 9.1.2.  Interpolated QTRACER.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 QTRACER2. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER2.

Some difference will be noted between Figure 35 and Figure 17 (page 93), but not a significant difference. Interpolation results in more data points falling on the necessary straight line; the equation of the straight line has different values for the y intercept and slope. As such, a slightly different estimate for longitudinal dispersion results.

Table 12 compares the final analytical output for the unaltered BTC for the QTRACER.DAT data set, the interpolated QTRACER.DAT data set, and the Interpolated-extrapolated QTRACER.DAT data set. Note how each file's results are closely matched with the others.
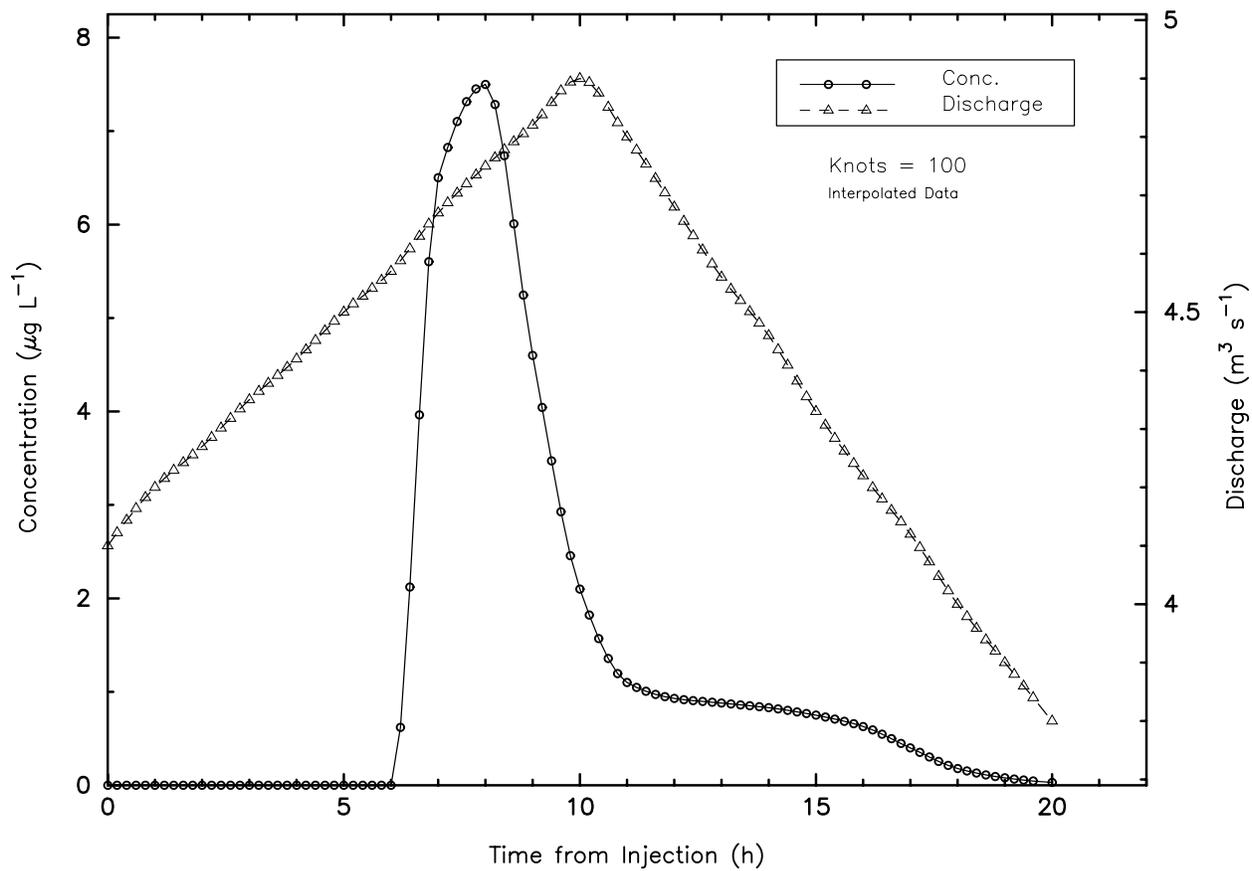
Figure 34. Interpolated curve for the QTRACER.DAT sampling station data file.

$$Y = \quad 875.168 + \quad -110.475 \; X$$

$R^2 = 0.9691$

$r = -.9844$

$z = -2.424$

PROB $= 0.5685E{-}11$

Chatwin Parameter

Y-axis: $[t \ln (A_p / C\sqrt{t})]^{1/2} \; (s^{1/2})$

X-axis: Time from Injection (h)
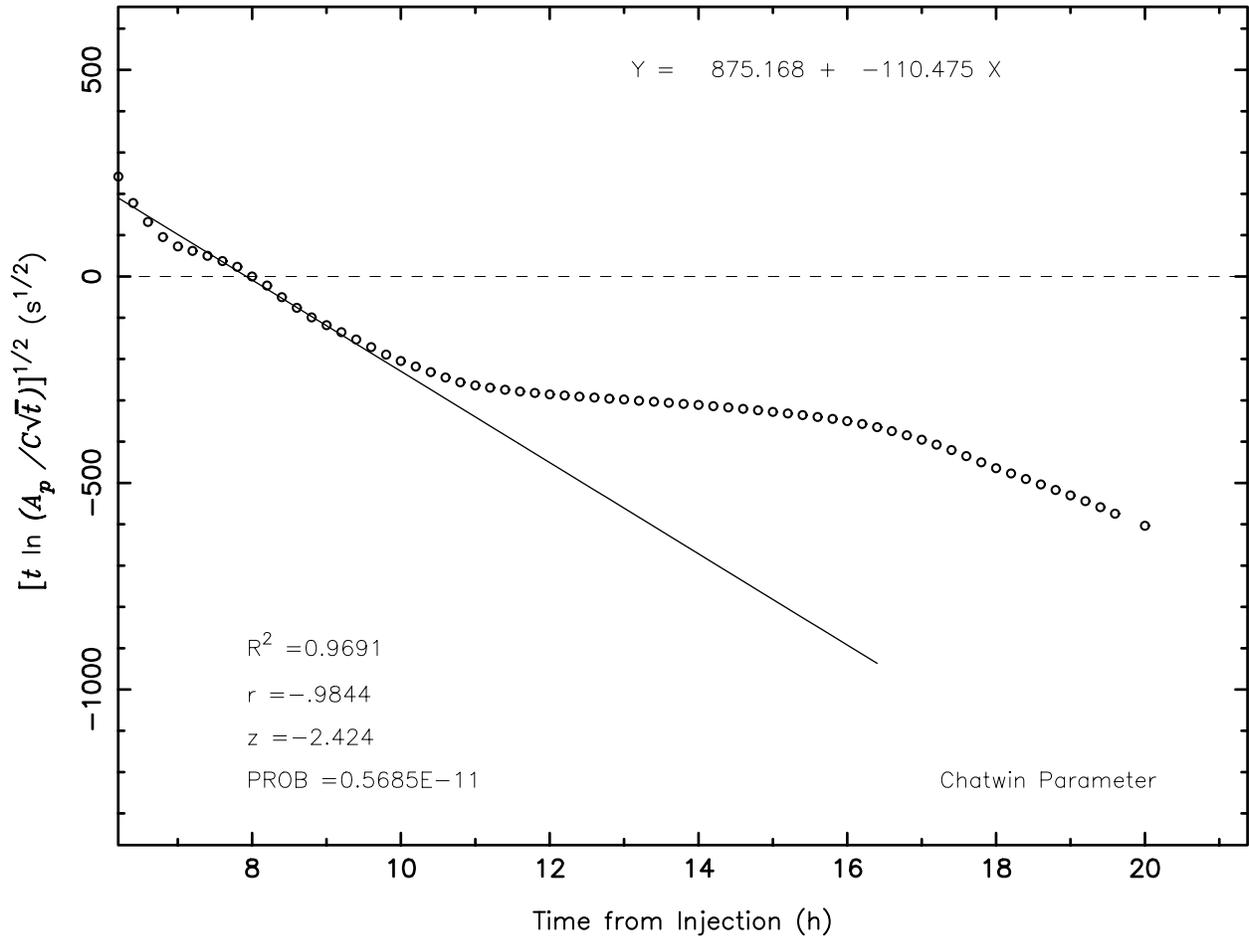
Figure 35. Interpolated data set for the Chatwin parameter for the QTRACER.DAT sampling station data file.

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Table 12. Estimated hydraulic flow and geometric parameters from BTCs for `QTRACER.DAT` sampling station.

| Parameter | QTRACER.DAT (unaltered) | QTRACER.DAT (interpolated) | QTRACER.DAT[1] (extrapolated) | QTRACER.DAT[2] (inter./extra.) |
|---|---|---|---|---|
| Tracer Mass Recovered, g | $4.48 \times 10^2$ | $4.48 \times 10^2$ | $4.48 \times 10^2$ | $4.48 \times 10^2$ |
| Percent Mass Recovered | $9.96 \times 10^1$ | $9.95 \times 10^1$ | $9.96 \times 10^1$ | $9.96 \times 10^1$ |
| Accuracy Index | $4.48 \times 10^{-3}$ | $4.75 \times 10^{-3}$ | $3.67 \times 10^{-3}$ | $3.80 \times 10^{-3}$ |
| Initial Tracer Breakthrough, h | $7.00 \times 10^0$ | $6.20 \times 10^0$ | $7.00 \times 10^0$ | $6.10 \times 10^0$ |
| Time to Peak Concentration, h | $8.00 \times 10^0$ | $8.00 \times 10^0$ | $8.00 \times 10^0$ | $8.00 \times 10^0$ |
| Mean Tracer Residence Time, h | $9.27 \times 10^0$ | $9.26 \times 10^0$ | $9.28 \times 10^0$ | $9.27 \times 10^0$ |
| Elapsed Tracer Travel Time, h | $2.00 \times 10^1$ | $2.00 \times 10^1$ | $2.26 \times 10^1$ | $2.32 \times 10^1$ |
| Maximum Tracer Flow Velocity, m h$^{-1}$ | $3.86 \times 10^2$ | $4.36 \times 10^2$ | $3.86 \times 10^2$ | $4.43 \times 10^2$ |
| Peak Tracer Flow Velocity, m h$^{-1}$ | $3.38 \times 10^2$ | $3.38 \times 10^2$ | $3.38 \times 10^2$ | $3.38 \times 10^2$ |
| Mean Tracer Flow Velocity, m h$^{-1}$ | $2.91 \times 10^2$ | $2.92 \times 10^2$ | $2.91 \times 10^2$ | $2.91 \times 10^2$ |
| Shear Velocity, m h$^{-1}$ | $6.12 \times 10^1$ | $6.13 \times 10^1$ | $6.12 \times 10^1$ | $6.12 \times 10^1$ |
| Longitudinal Dispersion, m$^2$ h$^{-1}$ | $1.17 \times 10^4$ | $8.57 \times 10^3$ | $1.17 \times 10^4$ | $7.68 \times 10^3$ |
| Hydraulic Head Loss, m | $1.21 \times 10^{-2}$ | $1.21 \times 10^{-2}$ | $1.21 \times 10^{-2}$ | $1.21 \times 10^{-2}$ |

Table 12. Estimated hydraulic flow and geometric parameters from BTCs for `QTRACER.DAT` sampling station (*continued*).

| Parameter | QTRACER.DAT (unaltered) | QTRACER.DAT (interpolated) | QTRACER.DAT[1] (extrapolated) | QTRACER.DAT[2] (inter./extra.) |
|---|---|---|---|---|
| Flow-Channel Volume, $m^3$ | $1.49 \times 10^5$ | $1.49 \times 10^5$ | $1.50 \times 10^3$ | $1.50 \times 10^3$ |
| Flow-Channel Cross-Sectional Area, $m^2$ | $5.53 \times 10^1$ | $5.53 \times 10^1$ | $5.54 \times 10^1$ | $5.54 \times 10^1$ |
| Flow-Channel Surface Area, $m^2$ | $5.17 \times 10^7$ | $5.17 \times 10^7$ | $5.16 \times 10^7$ | $5.17 \times 10^7$ |
| Tracer Sorption Coefficient, m | $1.30 \times 10^{-5}$ | $1.38 \times 10^{-5}$ | $1.07 \times 10^{-5}$ | $1.10 \times 10^{-5}$ |
| Tube Diameter, m | $8.39 \times 10^0$ | $8.39 \times 10^0$ | $8.40 \times 10^0$ | $8.40 \times 10^0$ |
| Hydraulic Depth, m | $6.59 \times 10^0$ | $6.59 \times 10^0$ | $6.60 \times 10^0$ | $6.59 \times 10^0$ |
| Friction Factor | $1.13 \times 10^{-1}$ | $1.13 \times 10^{-1}$ | $1.13 \times 10^{-1}$ | $1.13 \times 10^{-1}$ |
| Viscous-Flow Sublayer, m | $1.38 \times 10^{-3}$ | $1.38 \times 10^{-3}$ | $1.38 \times 10^{-3}$ | $1.38 \times 10^{-3}$ |
| Reynolds Number | $5.96 \times 10^5$ | $5.96 \times 10^5$ | $5.95 \times 10^5$ | $5.96 \times 10^5$ |
| Froude Number | $1.01 \times 10^{-2}$ | $1.01 \times 10^{-2}$ | $1.01 \times 10^{-2}$ | $1.01 \times 10^{-2}$ |
| Péclet Number | $6.70 \times 10^1$ | $9.19 \times 10^1$ | $6.70 \times 10^1$ | $1.02 \times 10^2$ |
| Schmidt Number | $1.14 \times 10^3$ | $1.14 \times 10^3$ | $1.14 \times 10^3$ | $1.14 \times 10^3$ |

Table 12. Estimated hydraulic flow and geometric parameters from BTCs for `QTRACER.DAT` sampling station (*continued*).

| Parameter | QTRACER.DAT (unaltered) | QTRACER.DAT (interpolated) | QTRACER.DAT[1] (extrapolated) | QTRACER.DAT[2] (inter./extra.) |
|---|---|---|---|---|
| Sherwood Number | $1.49 \times 10^4$ | $1.49 \times 10^4$ | $1.49 \times 10^4$ | $1.49 \times 10^4$ |
| Mass Transfer Coefficient, m s$^{-1}$ | $1.78 \times 10^{-6}$ | $1.78 \times 10^{-6}$ | $1.78 \times 10^{-6}$ | $1.78 \times 10^{-2}$ |
| Molecular diffusion layer, m | $5.62 \times 10^{-4}$ | $5.62 \times 10^{-4}$ | $5.63 \times 10^{-4}$ | $5.63 \times 10^{-4}$ |

Listed parameters without dimensions are dimensionless.

[1]Extrapolated using a statistical straight line fit.

[2]Extrapolated using a cubic Hermite function.

### 9.1.3. Extrapolated QTRACER.DAT BTC

Figure 36 depicts the extrapolated BTC generated and analyzed by QTRACER2. Note that discharge has an interpolated value for each time an extrapolated tracer concentration value is created.

Graphically, the user will note that the BTC shown in Figure 36 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 data point (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 36). Extrapolation routine 2 (piecewise cubic Hermite) uses the shape of the entire existing data curve to determine the "most reasonable" extrapolation data point 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 is measured, QTRACER2 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.

### 9.1.4. Extrapolated QTRACER.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 QTRACER2. Note that the straight-line fit, the equation for the straight line, and the relevant statistics describing the straight-line fit generated by QTRACER2 are identical to Figure 17. Data extrapolation had no effect on the Chatwin method analysis because the original sample had resulted in nearly "complete" tracer recovery.

### 9.2. INTERPOLATED-EXTRAPOLATED QTRACER.DAT DATA

Figures 38 and 39 illustrate how the interpolation and extrapolation routines provided in QTRACER2 can be used in BTC analyses. Table 12 illustrates that there are no significant differences in any of the analyses provided by QTRACER2 for the `QTRACER.DAT` data set.
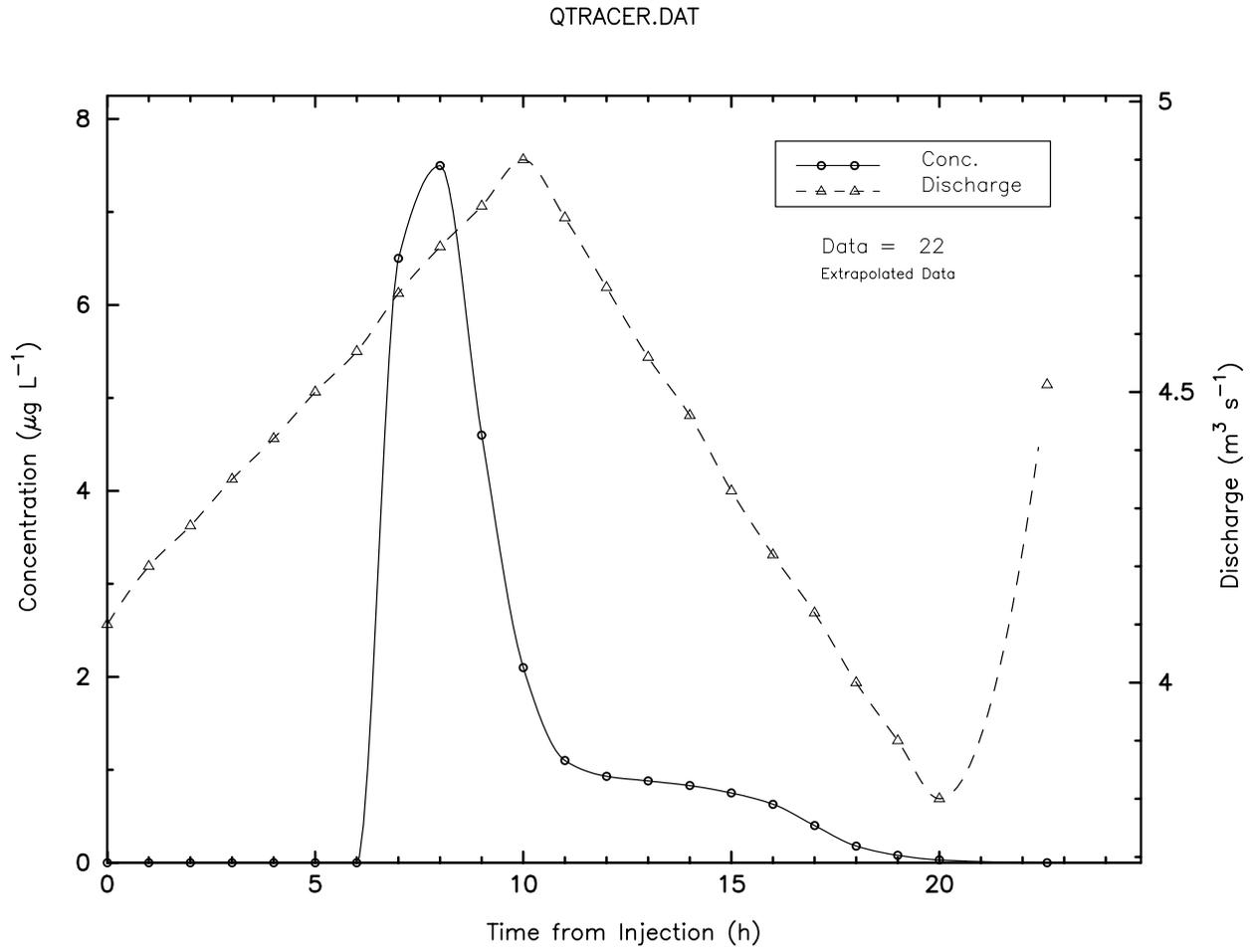
Figure 36. Extrapolated curve for the QTRACER.DAT sampling station data file.
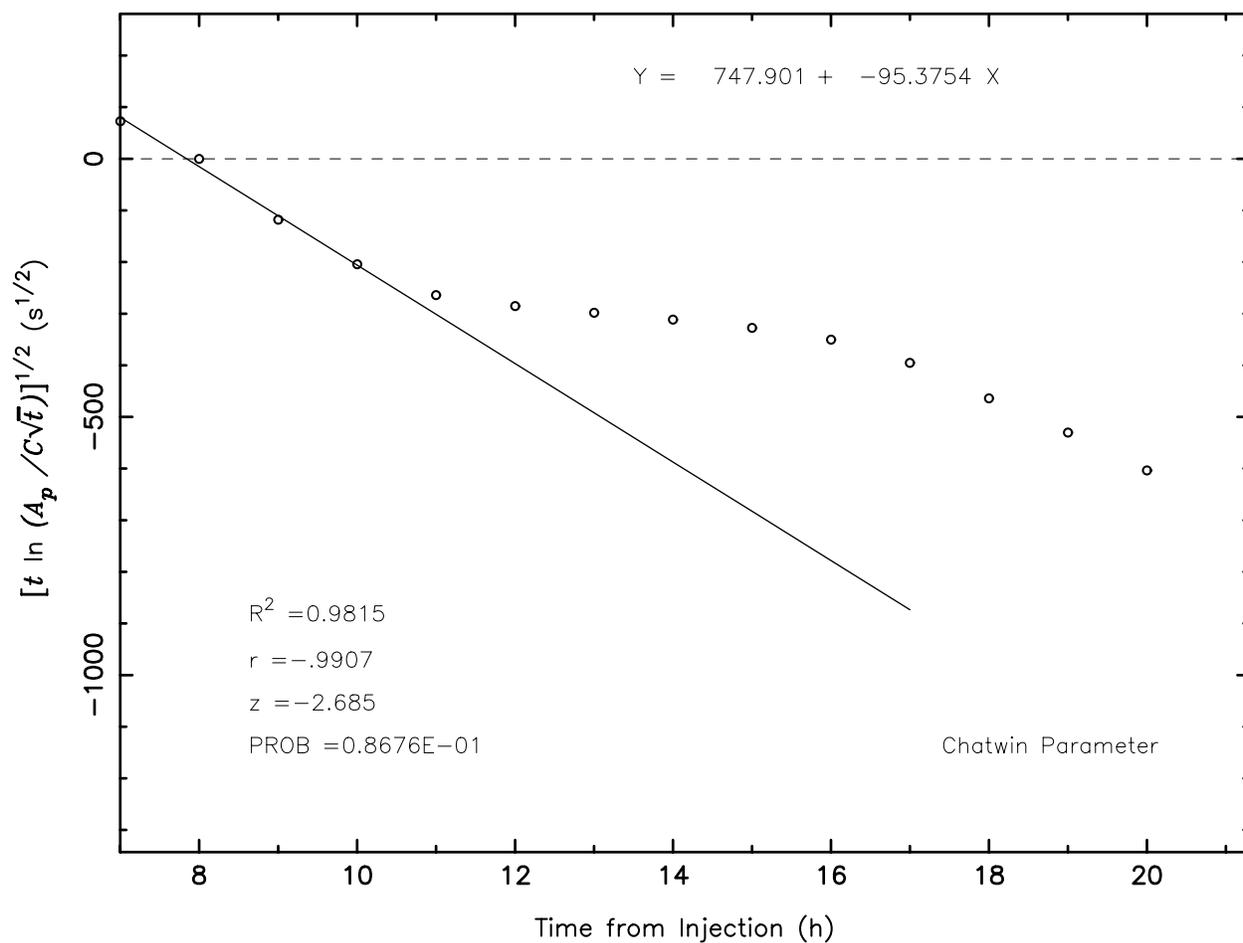
Figure 37. Extrapolated data set for the Chatwin parameter for the `QTRACER.DAT` sampling station data file.
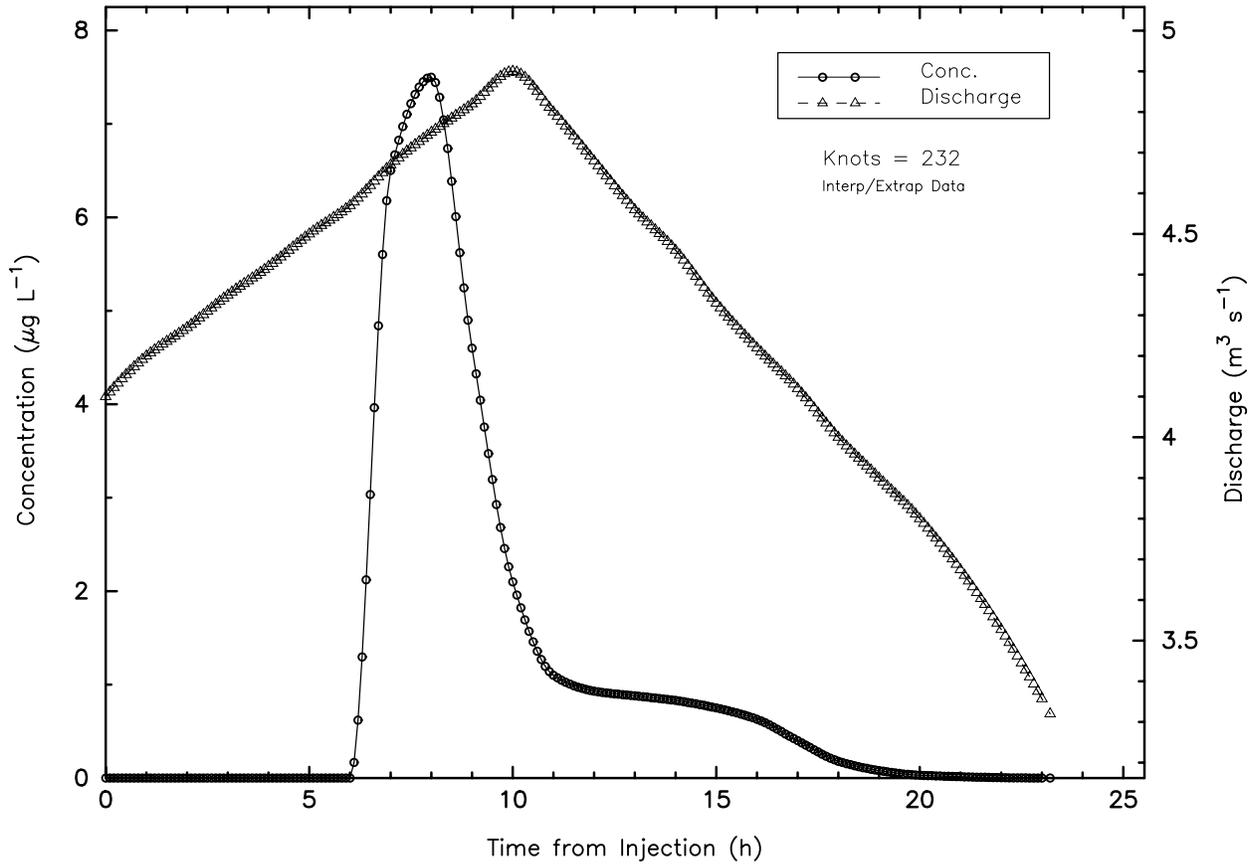
Figure 38. Interpolated and extrapolated data set for the QTRACER.DAT sampling station data file.

$Y = 924.127 + -116.842\ X$

$R^2 = 0.9236$

$r = -.9610$

$z = -1.959$

$PROB = 0.6660E-14$
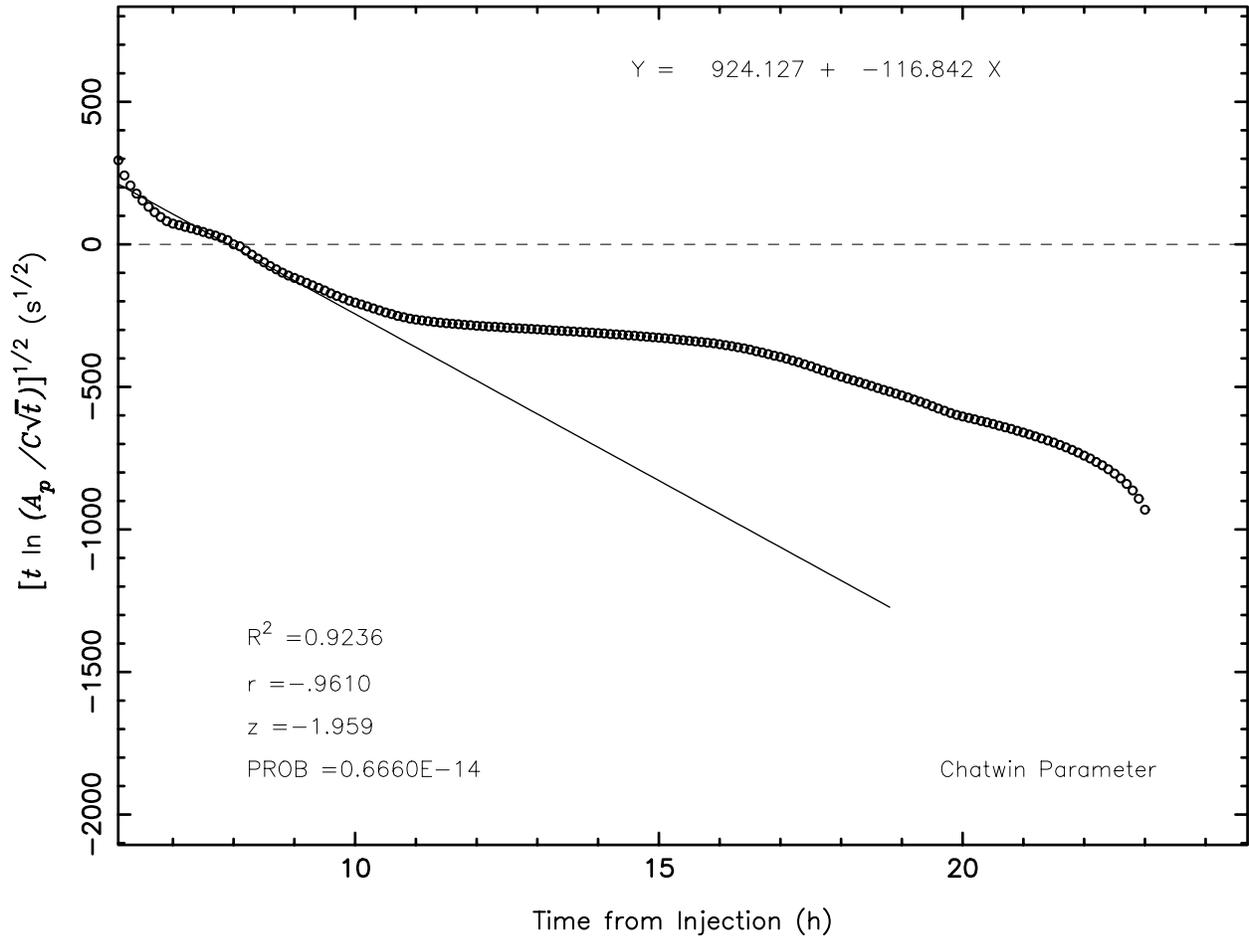
Chatwin Parameter

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

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A more erratic BTC, 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 are employed without data interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured data point to the extrapolated data point). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER2 will develop a smooth curve between all provided data points regardless of BTC appearance.

## 9.3.   COMPARISON OF RCA.DAT OUTPUT FILES

To further illustrate the effect of data interpolation, data extrapolation, and the combined effects of both 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.

### 9.3.1.   Interpolated RCA.DAT BTC

Figure 40 depicts the interpolated BTC generated and analyzed by QTRACER2. 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 40 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 data point. 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 QTRACER2.

### 9.3.2.   Interpolated RCA.DAT Chatwin Plot

Figure 41 depicts the interpolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER2. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER2.

Some difference will be noted between Figure 41 and Figure 23, but not a greatly significant difference. Interpolation results in more data points 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.

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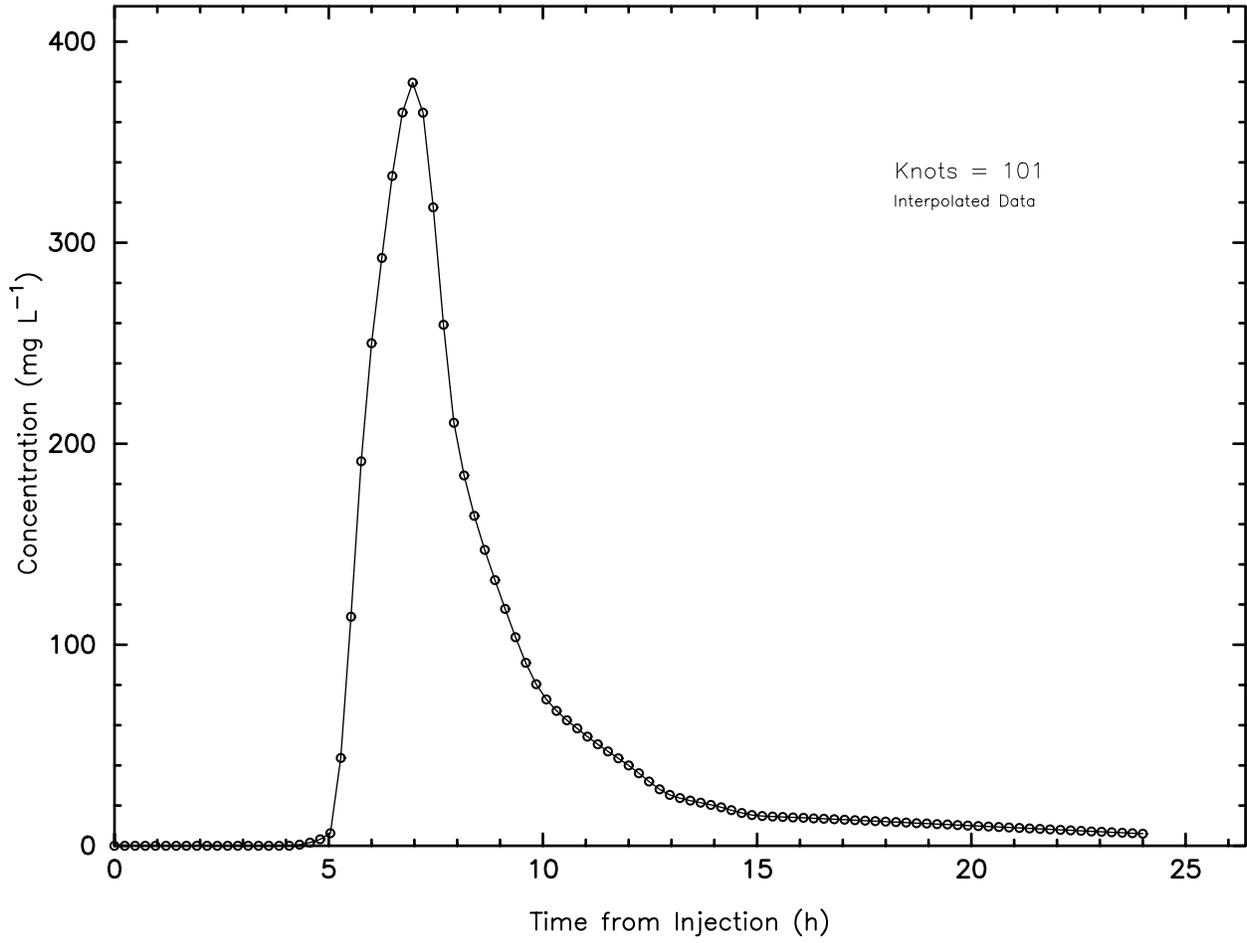
Figure 40. Interpolated curve for the RCA.DAT sampling station data file.
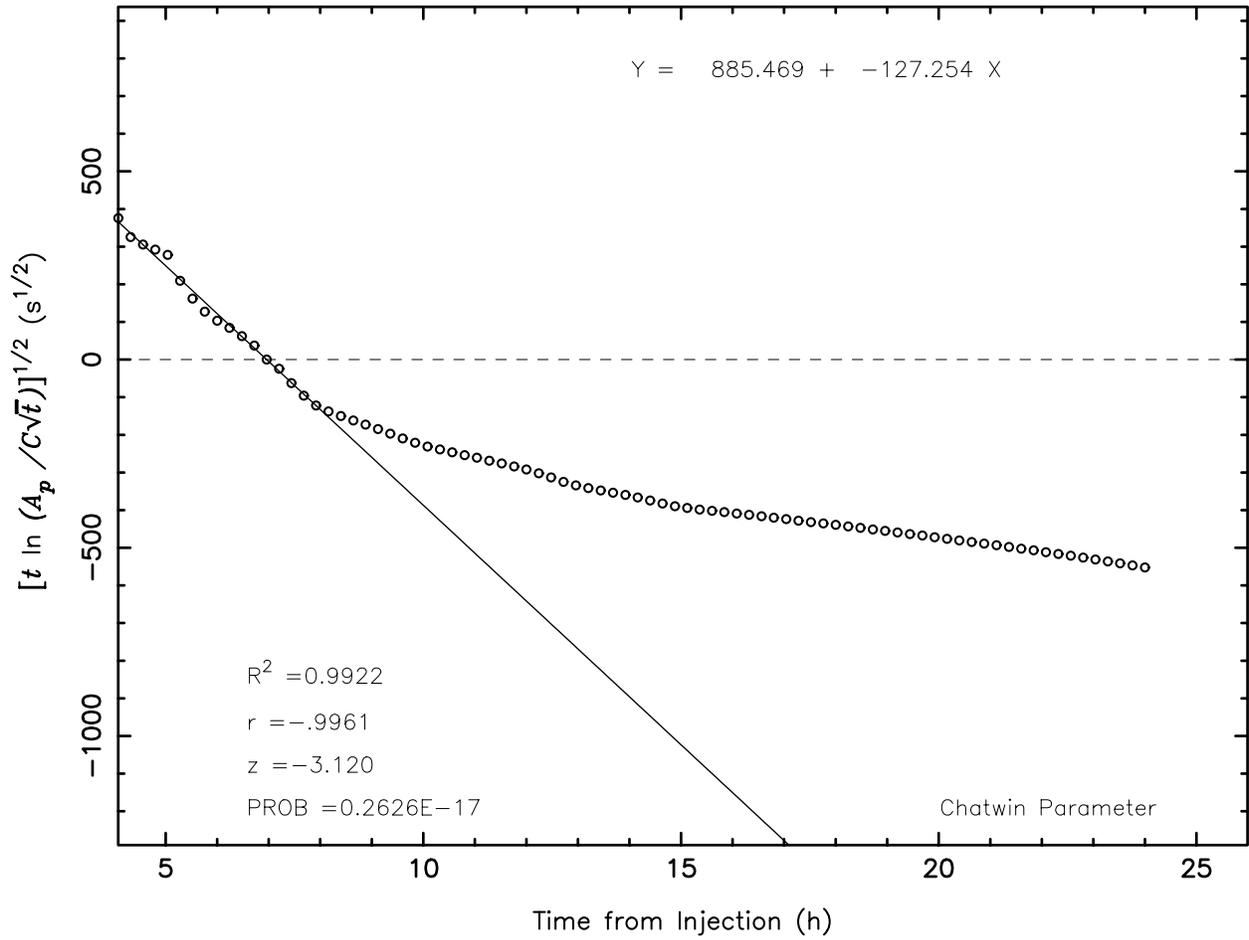
Figure 41. Interpolated data set for the Chatwin parameter for the `RCA.DAT` sampling station data file.

Table 13. Estimated hydraulic flow and geometric parameters from BTCs 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 | $1.74 \times 10^3$ | $1.74 \times 10^3$ | $1.77 \times 10^3$ | $1.77 \times 10^3$ |
| Percent Mass Recovered | $6.59 \times 10^{-1}$ | $6.59 \times 10^{-1}$ | $6.70 \times 10^{-1}$ | $6.71 \times 10^1$ |
| Accuracy Index | $9.93 \times 10^{-1}$ | $9.93 \times 10^{-1}$ | $9.93 \times 10^{-1}$ | $9.93 \times 10^{-1}$ |
| Initial Tracer Breakthrough, h | $5.00 \times 10^0$ | $4.08 \times 10^0$ | $5.00 \times 10^0$ | $4.08 \times 10^0$ |
| Time to Peak Concentration, h | $7.00 \times 10^0$ | $6.96 \times 10^0$ | $7.00 \times 10^0$ | $6.96 \times 10^0$ |
| Mean Tracer Residence Time, h | $8.61 \times 10^0$ | $8.60 \times 10^0$ | $8.90 \times 10^0$ | $8.95 \times 10^0$ |
| Elapsed Tracer Travel Time, h | $2.40 \times 10^1$ | $2.40 \times 10^1$ | $3.17 \times 10^1$ | $5.20 \times 10^1$ |
| Maximum Tracer Flow Velocity, m h$^{-1}$ | $6.71 \times 10^0$ | $8.22 \times 10^0$ | $6.71 \times 10^0$ | $8.22 \times 10^0$ |
| Peak Tracer Flow Velocity, m h$^{-1}$ | $4.79 \times 10^0$ | $4.82 \times 10^0$ | $4.79 \times 10^0$ | $4.82 \times 10^0$ |
| Mean Tracer Flow Velocity, m h$^{-1}$ | $3.91 \times 10^0$ | $3.91 \times 10^0$ | $3.78 \times 10^0$ | $3.76 \times 10^0$ |
| Shear Velocity, m h$^{-1}$ | $7.77 \times 10^{-1}$ | $7.77 \times 10^{-1}$ | $7.58 \times 10^{-1}$ | $7.55 \times 10^{-1}$ |
| Longitudinal Dispersion, m$^2$ s$^{-1}$ | $1.15 \times 10^0$ | $1.29 \times 10^0$ | $1.15 \times 10^0$ | $1.38 \times 10^0$ |
| Hydraulic Head Loss, m | $3.04 \times 10^{-7}$ | $3.04 \times 10^{-7}$ | $2.85 \times 10^{-7}$ | $2.81 \times 10^{-7}$ |
| Flow-Channel Volume, m$^3$ | $1.17 \times 10^1$ | $1.17 \times 10^1$ | $1.21 \times 10^1$ | $1.22 \times 10^1$ |
| Flow-Channel Cross-Sectional Area, m$^2$ | $3.50 \times 10^{-1}$ | $3.50 \times 10^{-1}$ | $3.62 \times 10^{-1}$ | $3.64 \times 10^{-1}$ |
| Flow-Channel Surface Area, m$^2$ | $2.12 \times 10^4$ | $2.12 \times 10^4$ | $2.11 \times 10^4$ | $2.10 \times 10^4$ |
| Tracer Sorption Coefficient, m | $8.32 \times 10^{-2}$ | $8.32 \times 10^{-2}$ | $8.53 \times 10^{-2}$ | $8.57 \times 10^{-2}$ |
| Tube Diameter, m | $6.67 \times 10^{-1}$ | $6.67 \times 10^{-1}$ | $6.79 \times 10^{-1}$ | $6.80 \times 10^{-1}$ |

Table 13. Estimated hydraulic flow and geometric parameters from BTCs for `RCA.DAT` sampling station (*continued*).

| Parameter | RCA.DAT (unaltered) | RCA.DAT (interpolated) | RCA.DAT[1] (extrapolated) | RCA.DAT[2] (inter./extra.) |
|---|---|---|---|---|
| Friction Factor | $1.01 \times 10^{-1}$ | $1.01 \times 10^{-1}$ | $1.02 \times 10^{-1}$ | $1.03 \times 10^{-1}$ |
| Laminar Hydraulic Conductivity, m s$^{-1}$ | $1.20 \times 10^{5}$ | $1.20 \times 10^{5}$ | $1.24 \times 10^{5}$ | $1.25 \times 10^{5}$ |
| Reynolds Number | $6.35 \times 10^{2}$ | $6.35 \times 10^{2}$ | $6.25 \times 10^{2}$ | $6.23 \times 10^{2}$ |
| Froude Number | $4.79 \times 10^{-4}$ | $4.79 \times 10^{-4}$ | $4.59 \times 10^{-4}$ | $4.56 \times 10^{-4}$ |
| Péclet Number | $1.14 \times 10^{2}$ | $1.02 \times 10^{2}$ | $1.10 \times 10^{2}$ | $9.16 \times 10^{1}$ |
| Schmidt Number | $1.14 \times 10^{3}$ | $1.14 \times 10^{3}$ | $1.14 \times 10^{3}$ | $1.14 \times 10^{3}$ |
| Sherwood Number | $1.40 \times 10^{2}$ | $1.40 \times 10^{2}$ | $1.40 \times 10^{2}$ | $1.40 \times 10^{2}$ |
| Mass Transfer Coefficient, m s$^{-1}$ | $2.09 \times 10^{-7}$ | $2.09 \times 10^{-7}$ | $2.06 \times 10^{-7}$ | $2.05 \times 10^{-2}$ |
| Molecular diffusion layer, m | $4.78 \times 10^{-3}$ | $4.78 \times 10^{-3}$ | $4.86 \times 10^{-3}$ | $4.87 \times 10^{-3}$ |

Listed parameters without dimensions are dimensionless.

[1]Extrapolated using a statistical straight line fit.

[2]Extrapolated using a cubic Hermite function.

Table 13 compares the final analytical output for the unaltered BTC 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.

### 9.3.3. Extrapolated RCA.DAT BTC

Figure 42 depicts the extrapolated BTC generated and analyzed by QTRACER2. Note that discharge has no extrapolated value because discharge was constant.

Graphically, the user will note that Figure 42 is more reasonable than Figure 22. The improvement is most evident in 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 42 suggests nearly "complete" tracer recovery at $> 30$ hours.
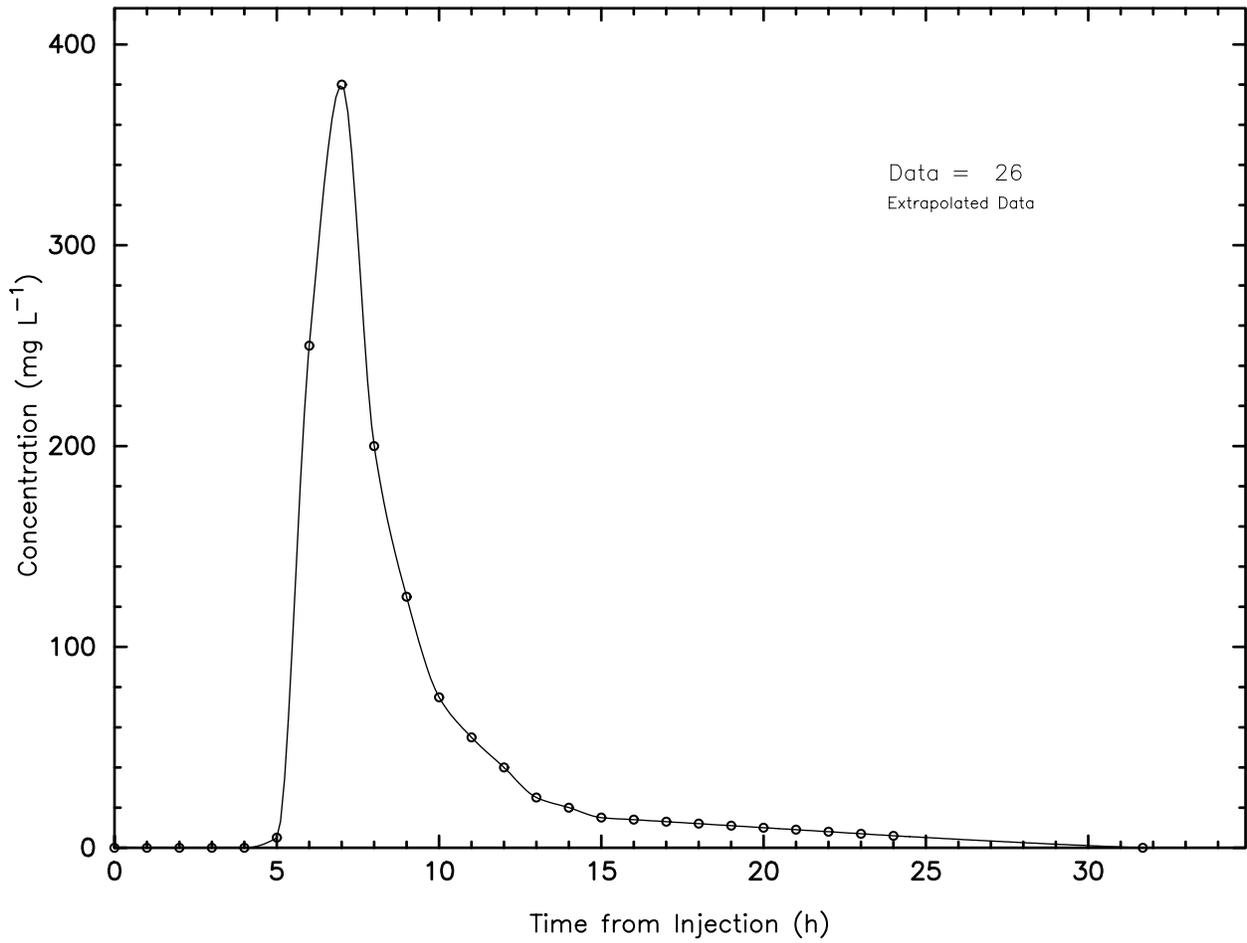
Figure 42. Extrapolated curve for the `RCA.DAT` sampling station data file.

### 9.3.4. Extrapolated RCA.DAT Chatwin Plot

Figure 43 depicts the extrapolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER2. Note that the straight-line fit, equation for the straight-line, and relevant statistics describing the straight-line fit generated by QTRACER2 are slightly different from the results shown in Figure 23.

The obvious differences between Figure 43 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 straight-line fit to the data that is not as good.

### 9.4. INTERPOLATED-EXTRAPOLATED RCA.DAT DATA

Figures 44 and 45 illustrate how the interpolation and extrapolation routines provided in QTRACER2 can be used in BTC analyses. Table 13 illustrates that there are no significant differences in any of the analyses provided by QTRACER2 for the RCA.DAT data set.

The user will note in Figure 44 that the exponential decay equation

$$y = 660.115 \, e^{-0.215973x} \tag{77}$$

has been produced along with the correlation coefficient $r$ (-0.9418) and the standard error of the estimated fit (50.87). QTRACER2 provides this information to the user to assist in assessing the effect of an exponential decay on a BTC. Whereas extrapolation methods 2 (piecewise cubic Hermite) and 3 (statistical method) produce a single extrapolated point, method 1 (exponential decay) produces five additional data points and thus has a great deal more influence on the final results.

Exponential decay extrapolation has more influence because the integration routine employed by QTRACER2 is forced to conform to the shape of the exponentially decaying curve. It is therefore incumbent upon the user to determine how appropriate it is to use an exponential decay model for extrapolation. For example, applying an exponential decay model for extrapolation to the QTRACER.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 BTC 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 are employed. The user should note that when data extrapolation is employed without data

$$Y = 937.976 + -134.329\ X$$

$R^2 = 0.9867$

$r = -.9933$

$z = -2.850$

$PROB = 0.6665E-02$

Chatwin Parameter

y-axis: $[t \ln (A_p /C\sqrt{t})]^{1/2}$ $(s^{1/2})$

x-axis: Time from Injection (h)
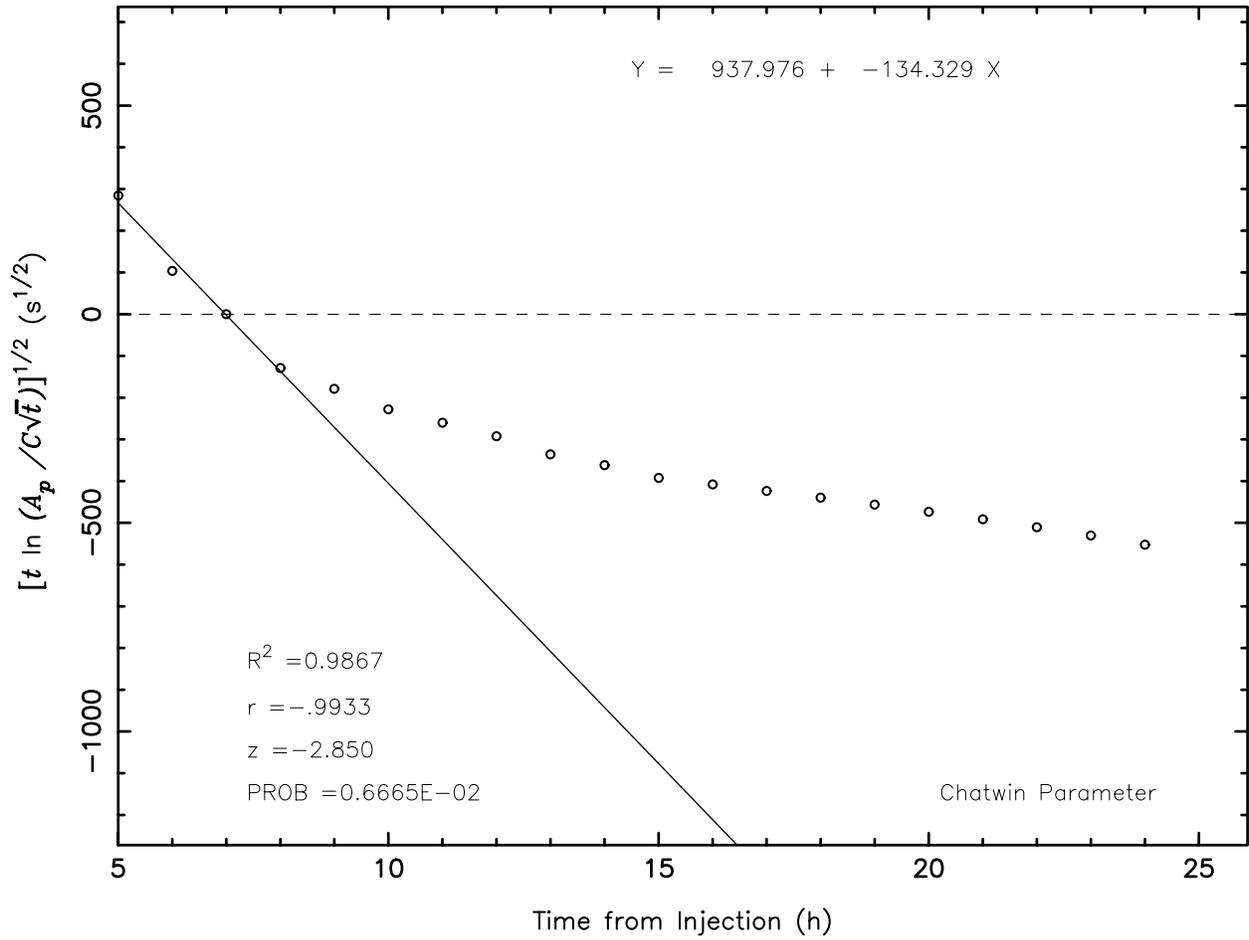
Figure 43. Extrapolated data set for the Chatwin parameter for the RCA.DAT sampling station data file.
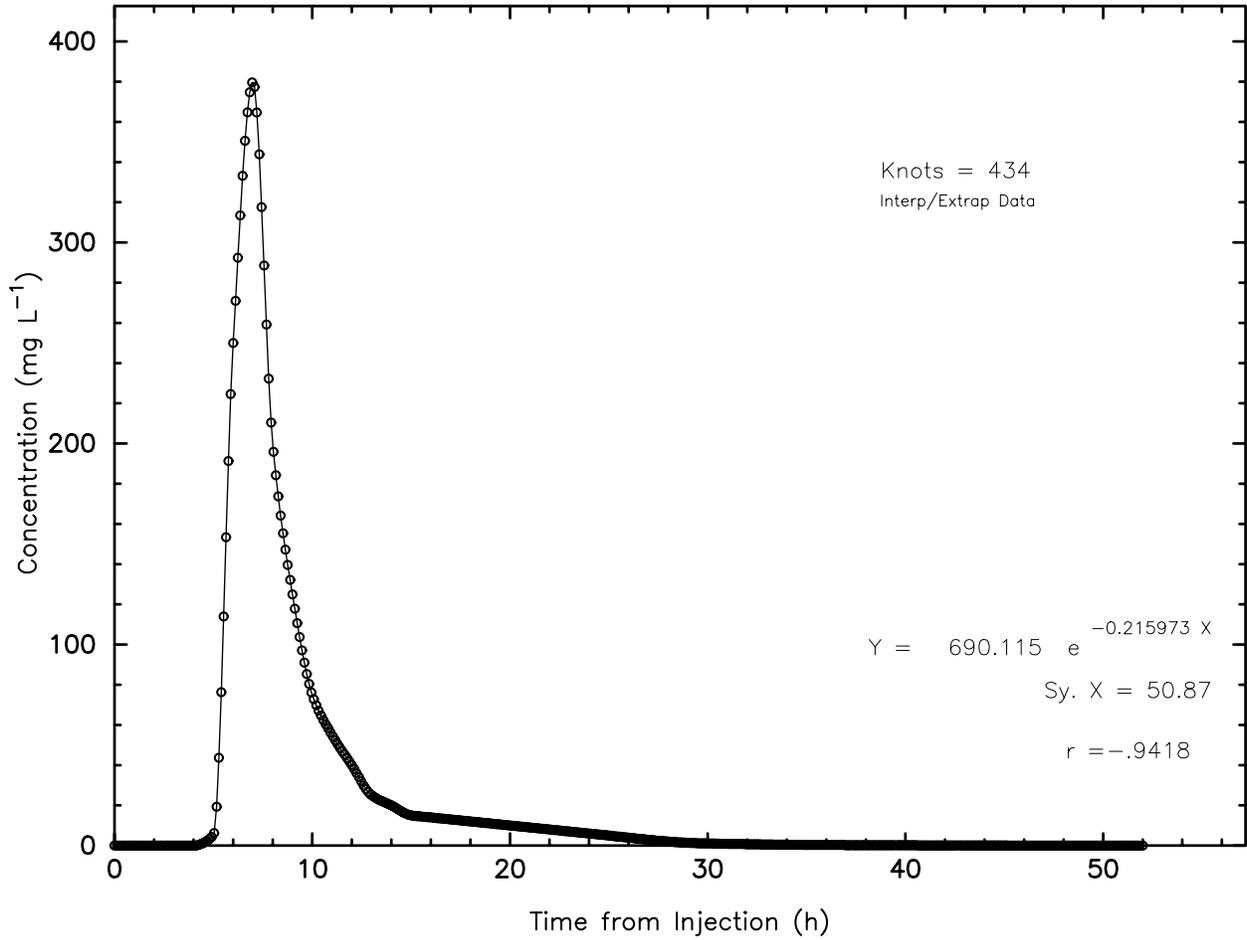
Figure 44. Interpolated and extrapolated data set for the RCA.DAT sampling station data file.
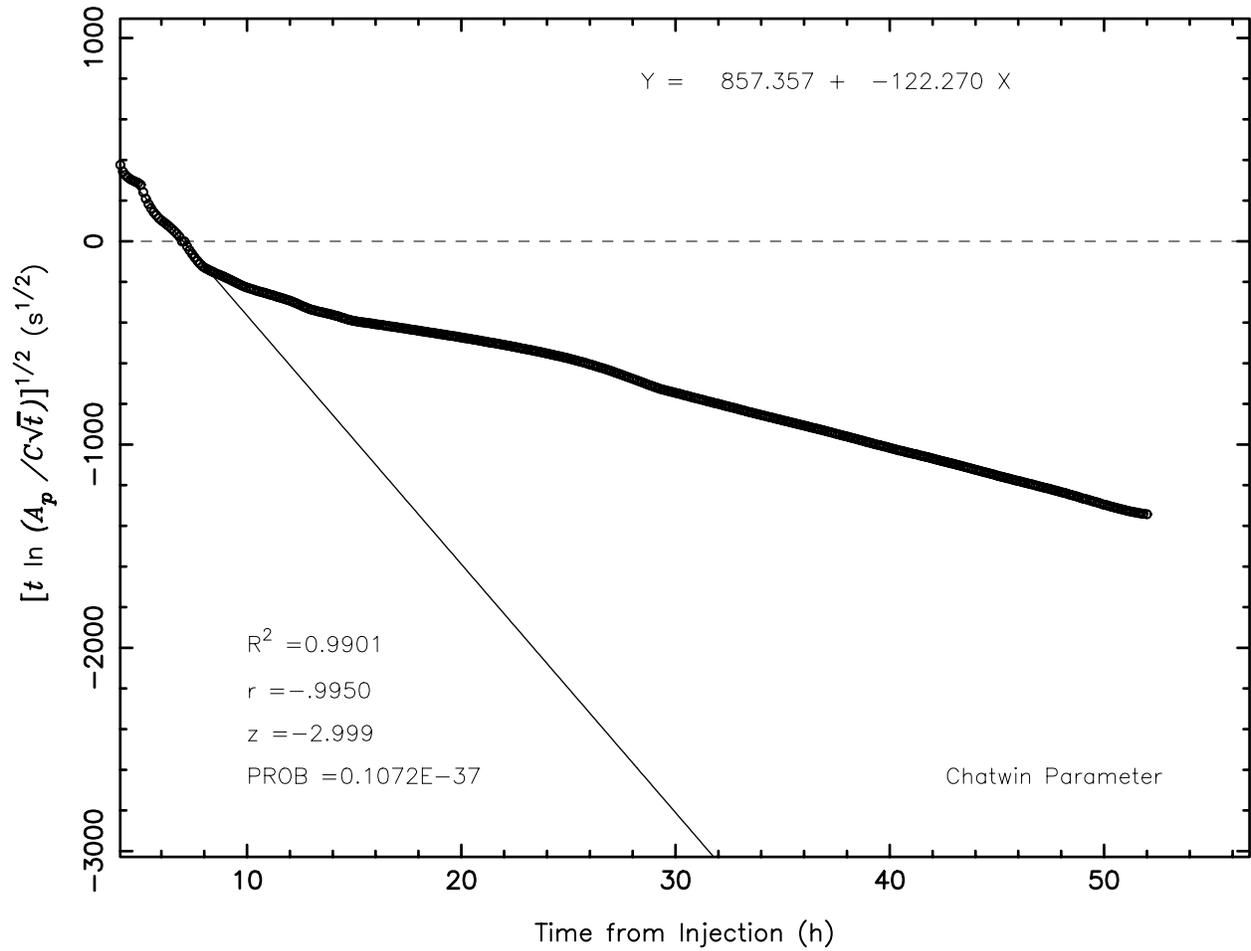
Figure 45. Interpolated and extrapolated data for the Chatwin parameter for `RCA.DAT` sampling station data file.

interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured data point to the extrapolated data point). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER2 will develop a smooth curve between all provided data points regardless of BTC appearance.

# 10. ASSOCIATED COMPUTER PROGRAMS

To facilitate the efficient use of QTRACER2, 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 QTRACER2. The third program, DATFILE, provides a straightforward interface for the creation of a sample station data file.

The results of these three programs are easily appended or copied to a `*.DAT` file (see Section 6.6.24. on page 88 and the end of Figure 15). By judicious use of these programs, QTRACER2 can be made more efficient because the data can be quickly and easily placed in required form.

## 10.1. 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
```

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, NDATA.EXE, a very good data interpolation algorithm has been programmed (it is the same one used in QTRACER2). To use this program, *Left Double-Click* on `NDATA` and follow the instructions. Note that this program ONLY works on a time-concentration file or time-discharge file without any other headers. The algorithm must therefore be used on the original data set(s) and the results copied to the bottom of the final data file to be processed.

When using NDATA only X/Y data is recognized 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 the concentration value corresponds to time=15.0, the user would exclude the entire line from the data set to be processed. 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 QTRACER2 to perform data interpolation on a complete data file.

### 10.1.1. 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.

## 10.2. 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 that shown in Figure 46.

*Left Double-Click* `AUTOTIME` and then follow the instructions to create a new file of time-concentration data that can then be copied to the end of a `*.DAT` file and read by QTRACER2. 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 46 for conversion to decimal hours will result the file listed in Figure 47. As stated previously, that QTRACER2 allows for free-format data entry, so a nicely formatted data column is unnecessary. All that is necessary is that the two data columns be separated by at least one blank space or a comma.

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

```
 0.0000  0.0100  0.0323
11.5000  0.0100  0.0323
12.0000  0.0600  0.0323
12.5000  0.5000  0.0323
13.0000  1.3200  0.0323
13.5000  2.0500  0.0323
14.0000  3.9000  0.0323
14.5000  4.2000  0.0323
15.0000  4.2000  0.0323
15.5000  3.4000  0.0323
16.0000  3.0500  0.0323
16.5000  2.4500  0.0323
17.0000  2.0000  0.0323
17.5000  1.5000  0.0323
18.0000  1.2000  0.0323
18.5000  0.9500  0.0323
19.0000  0.8000  0.0323
19.5000  0.6000  0.0323
20.0000  0.5500  0.0323
20.5000  0.5000  0.0323
21.0000  0.4200  0.0323
21.5000  0.3700  0.0323
22.0000  0.3500  0.0323
22.5000  0.3000  0.0323
27.5000  0.2000  0.0323
36.5000  0.0100  0.0323
```

Figure 47. Example of a converted sample time-concentration file created by AUTOTIME (Mull et al., 1988).

## 10.3.  DATFILE COMPUTER PROGRAM

The easiest method for creating a sample station data file (Figure 15) may be accomplished by using a text 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. In addition, DATFILE may be used to read in a QTRACER file (either a `*.D` file or a `*.DAT` file) for quick conversion to a QTRACER2-readable file

To use DATFILE, the user need only *Left Double-Click* DATFILE and respond to each requestor in turn.  In the create mode, DATFILE only produces the upper portion of a sampling station data file.  The actual TIME CONCENTRATION DISCHARGE data must be appended to the end of the data file created by DATFILE. In the conversion mode, DATFILE attempts to automatically identify the type of file to be converted by recognizing the first word of the file (`QUANTITY` = `*.D` file; `SAMPLING` = `*.Dat` file).  If DATFILE cannot identify the file, the user is requested to provide identification for DATFILE. Upon recognition, the user then responds to a few appropriate requestors.

A sample station data file created or converted from a QTRACER-file form using DATFILE will not appear exactly in the form of Figure 15 because of some formatting differences. This is not a concern because QTRACER2 uses free format for input.

### 10.3.1.  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.

### 10.4.  COMBINE COMPUTER PROGRAM

Typically, as mentioned in Section 10.1. on page 154 discharge is not measured as frequently or at the same time as tracer concentration.  With the advent of continuous-flow filter fluorometers, pressure transducers, and data loggers, automatic data recording is now normally conducted.  However, if the time settings on these various instruments are not synchronized or one automatic recording device takes readings less frequently than the a different recording device, then use of QTRACER in which one "universal" set of TIME data is used is problematic.  For example, consider the following time-concentration data set (Combine1.dat; modified from the QTRACER.DAT file using the interpolation function of QTRACER) shown in Figure 48  and the time-discharge data set (Combine2.dat; unmodifed from the QTRACER.DAT file) shown in Figure 49.

```
0.000000000    0.000000000
0.2000000030   0.000000000
0.4000000060   0.000000000
0.6000000238   0.000000000
0.8000000119   0.000000000
1.000000000    0.000000000
1.200000048    0.000000000
1.399999976    0.000000000
1.600000024    0.000000000
1.799999952    0.000000000
2.000000000    0.000000000
2.200000048    0.000000000
2.400000095    0.000000000
2.599999905    0.000000000
2.799999952    0.000000000
3.000000000    0.000000000
3.200000048    0.000000000
3.399999857    0.000000000
3.599999905    0.000000000
3.799999952    0.000000000
4.000000000    0.000000000
4.199999809    0.000000000
4.399999619    0.000000000
4.599999905    0.000000000
4.799999714    0.000000000
5.000000000    0.000000000
5.199999809    0.000000000
5.399999619    0.000000000
5.599999905    0.000000000
5.799999714    0.000000000
6.000000000    0.000000000
6.199999809    0.6205322146
6.400000095    2.121600866
6.599999905    3.962399006
6.799999714    5.602131367
7.000000000    6.500000000
7.199999809    6.825866222
7.400000095    7.101600170
7.599999905    7.314399719
7.800000191    7.451466560
```

Figure 48. Example of a measured sample time-concentration file as recorded by an automatic data recorded (modified from the QTRACER.DAT).

```
 8.000000000    7.500000000
 8.199999809    7.284326077
 8.399999619    6.736979008
 8.599999428    6.007468700
 8.799999237    5.245306492
 9.000000000    4.599999905
 9.199999809    4.042011261
 9.399999619    3.470477104
 9.599999428    2.927937984
 9.799999237    2.456932783
 9.999999046    2.100001335
10.19999886     1.822443485
10.39999962     1.570183516
10.59999943     1.356703877
10.79999924     1.195482850
10.99999905     1.100000262
11.19999886     1.047596455
11.39999866     1.005732298
11.59999847     0.9730700850
11.79999924     0.9482718706
11.99999905     0.9300000668
12.19999886     0.9165091515
12.39999866     0.9060727954
12.59999847     0.8973819017
12.79999828     0.8891273141
12.99999809     0.8800001144
13.19999886     0.8703692555
13.39999866     0.8611077666
13.59999847     0.8516616225
13.79999828     0.8414769769
13.99999809     0.8300001025
14.19999790     0.8168752193
14.39999771     0.8021946549
14.59999847     0.7860764265
14.79999828     0.7686389089
14.99999809     0.7500001788
15.19999790     0.7302790880
15.39999771     0.7090768218
15.59999752     0.6857351661
15.79999733     0.6595957875
```

Figure 48.  Example of a measured sample time-concentration file as recorded by an automatic data recorded (modified from the QTRACER.DAT) (*continued*).

```
15.99999809      0.6300002933
16.19999695      0.5930896401
16.39999771      0.5479190350
16.59999847      0.4982038140
16.79999733      0.4476595819
16.99999809      0.4000004232
17.19999695      0.3527349830
17.39999771      0.3033765852
17.59999657      0.2556514442
17.79999733      0.2132840753
17.99999809      0.1800002754
18.19999695      0.1541337073
18.39999771      0.1314002424
18.59999657      0.1116003171
18.79999733      0.9453354031E-01
18.99999619      0.8000025153E-01
19.19999695      0.6706685573E-01
19.39999771      0.5520012602E-01
19.59999657      0.4480016232E-01
20.00000000      0.2999999933E-01
```

Figure 48. Example of a measured sample time-concentration file as recorded by an automatic data recorded (modified from the QTRACER.DAT) (*continued*).

```
 0.0   4.10
 1.0   4.20
 2.0   4.27
 3.0   4.35
 4.0   4.42
 5.0   4.50
 6.0   4.57
 7.0   4.67
 8.0   4.75
 9.0   4.82
10.0   4.90
11.0   4.80
12.0   4.68
13.0   4.56
14.0   4.46
15.0   4.33
16.0   4.22
17.0   4.12
18.0   4.00
19.0   3.90
20.0   3.80
```

Figure 49. Example of a measured sample time-discharge file as recorded by an automatic data recorded (unmodified from the QTRACER.DAT).

The two data files do not correspond because, assuming these appear as recorded by automatic recording devices, there are only 21 time-discharge data values, while there are 100 time-concentration data values. In this instance, each of the time values for the time-discharge data set has a matching time value in the time-concentration data set. However, even if there were no matching time values between the two disparate data sets, COMBINE would do a tolerable job of making a match.

To use COMBINE, the user need only start the program (*Left Double-Click* on the COMBINE icon) and select units for time, concentration, and discharge which can be arbitrary and are not necessary for the program to run. Next the user enters the time-concentration data file to be considered, then the time-discharge data file to be considered, then an output name for the resulting time-concentration-discharge data file, and a plot file name if a PostScript file of the screen plot is desired. A screen plot of the resulting time-concentration-discharge data file will be displayed *if* the chosen interpolation step is not too small. A selected interpolation step of 0.1 is recommended as an initial value, but the user is free to pretty much choose any value. However, a very small interpolation step (*e.g.*, 0.0001) will result in a massively huge file that may exceed the memory stack on the local computer.

Processing the two data files shown above, Combine1.dat and Combine2.dat, using COMBINE results in the following time-concentration-discharge data file shown in Figure 50.

### 10.4.1. COMBINE Screen Plotting

If the size of the created time-concentration-discharge file is of a reasonable size, COMBINE will display a screen plot from which a bitmapped file may be created. A screen plot was added so that the user may examine the results of the COMBINE-created file in relation to the original time-concentration and time-discharge data files. Although only a visual inpection, the screen plot allows the user the ability to verify that the COMBINE-created file is acceptable.

Figure 51 (page 169) depicts the results of Figure 50. The open circles in Figure 51 represent measured time-concentration data points from Figure 48 and the open triangles in Figure 51 represent measured time-discharge data points from Figure 49. The solid line in Figure 51 represents the interpolated time-concentration data shown in Figure 50 and the dashed line in Figure 51 represents the interpolated time-discharge data shown in Figure 50.

Although it is not readily apparent from Figure 51, the data listed in Figure 50 results

| TIME | CONCENTRATION | DISCHARGE |
|------|---------------|-----------|
| 0.0000000E+00 | 0.0000000E+00 | 4.100000 |
| 0.2000000 | 0.0000000E+00 | 4.122500 |
| 0.3000000 | 0.0000000E+00 | 4.133300 |
| 0.4000000 | 0.0000000E+00 | 4.143900 |
| 0.5000000 | 0.0000000E+00 | 4.154100 |
| 0.6000000 | 0.0000000E+00 | 4.164000 |
| 0.7000000 | 0.0000000E+00 | 4.173500 |
| 0.8000000 | 0.0000000E+00 | 4.182700 |
| 1.100000 | 0.0000000E+00 | 4.208000 |
| 1.200000 | 0.0000000E+00 | 4.215400 |
| 1.300000 | 0.0000000E+00 | 4.222500 |
| 1.400000 | 0.0000000E+00 | 4.229300 |
| 1.500000 | 0.0000000E+00 | 4.236000 |
| 1.600000 | 0.0000000E+00 | 4.242500 |
| 1.700000 | 0.0000000E+00 | 4.249100 |
| 1.800000 | 0.0000000E+00 | 4.255800 |
| 1.900000 | 0.0000000E+00 | 4.262700 |
| 2.000000 | 0.0000000E+00 | 4.270000 |
| 2.100000 | 0.0000000E+00 | 4.277600 |
| 2.200000 | 0.0000000E+00 | 4.285500 |
| 2.300000 | 0.0000000E+00 | 4.293600 |
| 2.400000 | 0.0000000E+00 | 4.301700 |
| 2.500000 | 0.0000000E+00 | 4.310000 |
| 2.600000 | 0.0000000E+00 | 4.318300 |
| 2.700000 | 0.0000000E+00 | 4.326400 |
| 2.800000 | 0.0000000E+00 | 4.334500 |
| 2.900000 | 0.0000000E+00 | 4.342400 |
| 3.000000 | 0.0000000E+00 | 4.350000 |
| 3.100000 | 0.0000000E+00 | 4.357300 |
| 3.200000 | 0.0000000E+00 | 4.364400 |
| 3.300000 | 0.0000000E+00 | 4.371400 |
| 3.400000 | 0.0000000E+00 | 4.378200 |
| 3.500000 | 0.0000000E+00 | 4.385000 |
| 3.600000 | 0.0000000E+00 | 4.391800 |
| 3.700000 | 0.0000000E+00 | 4.398600 |
| 3.800000 | 0.0000000E+00 | 4.405600 |
| 3.900000 | 0.0000000E+00 | 4.412700 |

Figure 50. Example of a converted sample time-concentration-discharge file created by COMBINE for use in QTRACER.

```
4.000000        0.0000000E+00        4.420000
4.100000        0.0000000E+00        4.427600
4.200000        0.0000000E+00        4.435500
4.300000        0.0000000E+00        4.443600
4.400000        0.0000000E+00        4.451700
4.500000        0.0000000E+00        4.460000
4.600000        0.0000000E+00        4.468300
4.700000        0.0000000E+00        4.476400
4.800000        0.0000000E+00        4.484500
4.900000        0.0000000E+00        4.492400
5.000000        0.0000000E+00        4.500000
5.100000        0.0000000E+00        4.507300
5.200000        0.0000000E+00        4.514200
5.300000        0.0000000E+00        4.520900
5.400000        0.0000000E+00        4.527500
5.500000        0.0000000E+00        4.534000
5.600000        0.0000000E+00        4.540700
5.700000        0.0000000E+00        4.547500
5.800000        0.0000000E+00        4.554600
5.900000        0.0000000E+00        4.562000
6.000000        0.0000000E+00        4.570000
6.100000        0.2003800            4.578700
6.200000        0.6203800            4.588100
6.300000        1.273800             4.598100
6.400000        2.121300             4.608500
6.500000        3.031500             4.619200
6.600000        3.962100             4.629900
6.700000        4.853700             4.640500
6.800000        5.601900             4.650900
6.900000        6.136200             4.660700
7.000000        6.499900             4.670000
7.100000        6.685300             4.678800
7.200000        6.825800             4.687300
7.300000        6.971000             4.695600
7.400000        7.101500             4.703800
7.500000        7.217100             4.711800
7.600000        7.314400             4.719600
7.700000        7.394800             4.727300
```

Figure 50. Example of a converted sample time-concentration-discharge file created by COMBINE for use in QTRACER (*continued*).

```
 7.800000        7.451500        4.735000
 7.900000        7.484700        4.742500
 8.000000        7.500000        4.750000
 8.100000        7.430900        4.757300
 8.200000        7.284400        4.764400
 8.300000        7.050300        4.771400
 8.400000        6.737100        4.778200
 8.500000        6.387400        4.785000
 8.600000        6.007600        4.791800
 8.700000        5.620800        4.798600
10.10000         1.955300        4.898200
10.20000         1.822500        4.893100
10.30000         1.692300        4.885300
10.40000         1.570300        4.875300
10.50000         1.457600        4.863600
10.60000         1.356800        4.850900
10.70000         1.268200        4.837600
10.80000         1.195500        4.824400
10.90000         1.141200        4.811600
11.00000         1.100000        4.800000
11.10000         1.071200        4.788900
11.20000         1.047600        4.777400
11.30000         1.025400        4.765600
11.40000         1.005700        4.753600
11.50000         0.9883500       4.741400
11.60000         0.9730800       4.729000
11.70000         0.9597900       4.716700
11.80000         0.9482800       4.704300
11.90000         0.9384500       4.692100
12.00000         0.9300100       4.680000
12.10000         0.9227900       4.667900
12.20000         0.9165100       4.655700
12.30000         0.9110100       4.643300
12.40000         0.9060800       4.631000
12.50000         0.9016000       4.618600
12.60000         0.8973800       4.606400
12.70000         0.8932800       4.594400
12.80000         0.8891300       4.582600
```

Figure 50. Example of a converted sample time-concentration-discharge file created by COMBINE for use in QTRACER (*continued*).

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```
12.90000          0.8846500          4.571100
13.00000          0.8800000          4.560000
13.10000          0.8752000          4.549400
13.20000          0.8703700          4.539300
13.30000          0.8657300          4.529500
13.40000          0.8611100          4.519900
13.50000          0.8564400          4.510500
13.60000          0.8516700          4.501000
13.70000          0.8467000          4.491300
13.80000          0.8414800          4.481400
13.90000          0.8359200          4.471000
14.00000          0.8300000          4.460000
14.10000          0.8236400          4.448300
14.20000          0.8168800          4.435800
14.30000          0.8097300          4.422800
14.40000          0.8022000          4.409400
14.50000          0.7943200          4.395800
14.60000          0.7860800          4.382100
14.70000          0.7775200          4.368500
14.80000          0.7686500          4.355200
14.90000          0.7594700          4.342300
15.00000          0.7500100          4.330000
15.10000          0.7403100          4.318200
15.20000          0.7302900          4.306700
15.30000          0.7199100          4.295300
15.40000          0.7090900          4.284200
15.50000          0.6977200          4.273200
15.60000          0.6857500          4.262400
15.70000          0.6730600          4.251700
15.80000          0.6596100          4.241000
15.90000          0.6454500          4.230500
16.00000          0.6300200          4.220000
16.10000          0.6125300          4.209700
16.20000          0.5931100          4.199700
16.30000          0.5713600          4.189900
16.40000          0.5479400          4.180200
16.50000          0.5234300          4.170500
16.60000          0.4982300          4.160900
```

Figure 50. Example of a converted sample time-concentration-discharge file created by COMBINE for use in QTRACER (*continued*).

```
16.70000          0.4728200          4.151000
16.80000          0.4476800          4.141000
16.90000          0.4236500          4.130700
17.00000          0.4000200          4.120000
17.10000          0.3764900          4.108800
17.20000          0.3527600          4.097000
17.30000          0.3281100          4.084900
17.40000          0.3034000          4.072500
17.50000          0.2790800          4.060000
17.60000          0.2556700          4.047500
17.70000          0.2335400          4.035100
17.80000          0.2133000          4.023000
17.90000          0.1956400          4.011200
18.00000          0.1800100          4.000000
18.10000          0.1664700          3.989300
18.20000          0.1541500          3.978800
18.30000          0.1424000          3.968700
18.40000          0.1314100          3.958700
18.50000          0.1211600          3.948900
18.60000          0.1116100          3.939100
18.70000          0.1027500          3.929400
18.80000          9.4541997E-02      3.919700
18.90000          8.7022997E-02      3.909900
19.00000          8.0007002E-02      3.900000
19.10000          7.3376998E-02      3.890000
19.20000          6.7073002E-02      3.880000
19.30000          6.0977999E-02      3.870000
19.40000          5.5206001E-02      3.860000
19.50000          4.9722001E-02      3.850000
19.60000          4.4805001E-02      3.840000
19.70000          4.0520001E-02      3.830000
19.80000          3.6550999E-02      3.820000
19.90000          3.3009000E-02      3.810000
20.00000          3.0003000E-02      3.800000
```

Figure 50. Example of a converted sample time-concentration-discharge file created by COMBINE for use in QTRACER (*continued*).
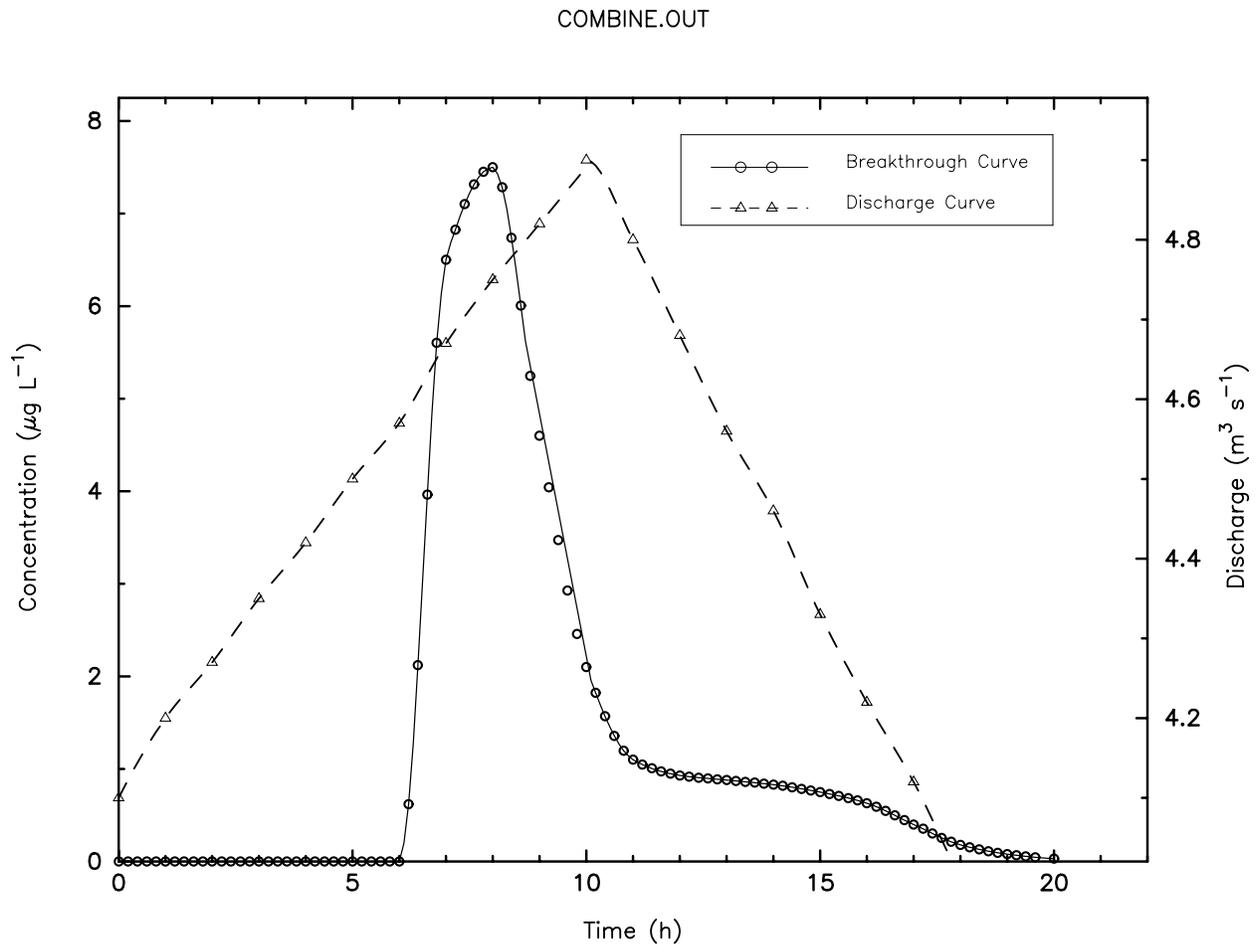
Figure 51. Plot of the Combine.out data listed in Figure 50.

in a very large file with a very small time spacing. This small time spacing results in a total of 185 data values (using a 0.1 interpolation step). Therefore, the solid and dashed lines actually plot as smooth curves rather than as a series of straight-line segments between data points. From this perspective the quality of the plot indicates that the data listed in Figure 50 would be acceptable for analysis by QTRACER.

### 10.4.2. COMBINE Processing

To be able to produce matching time-concentration and time-discharge data files COMBINE interpolates both data sets independently to produce two new, very large data files. These are then written to temporary storage and read back into the program in truncated form. The temporary storage can occupy considerable storage space so it is necessary that the user ensure that adequate storage space exists on the hard drive prior to running COMBINE.

By truncating the actual data, it is more likely that matching time values for the time-concentration and time-discharge data files will be obtained than if the entire data record were to be read. If the entire data record were to be read, it is probable that extraneous decimal places in the time-concentration and time-discharge data files could not be found to match. The new time-concentration-discharge file is then written to the hard drive and the temporary files deleted.

### 10.4.3. COMBINE Source

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

# 11.   CONCLUSIONS

Tracer-breakthrough curves developed from quantitative hydrological tracer tests can be evaluated given the present high level of accuracy of analytical fluorescence chemistry (and other tracer substances) 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, QTRACER2, 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. QTRACER2 will enhance the necessary analyses and lead to improved site evaluations.

# NOTATION

| | |
|---|---|
| $A$ | bulk flow region cross-sectional area ($L^2$) |
| $\mathbf{A}$ | matrix of time values used in the Chatwin analysis (T) |
| $A_I$ | accuracy index (dimensionless) |
| $A_p$ | constant of proportionality for amount of diffusing material (M T$^{1/2}$ L$^{-3}$) |
| $A_s$ | karst conduit surface ($L^2$) |
| $\mathbf{b}$ | vector of concentration parameters for the Chatwin analysis (T$^{1/2}$) |
| $C$ | tracer concentration (M L$^{-3}$) |
| $C_0$ | initial tracer concentration (M L$^{-3}$) |
| $\overline{C_b}$ | average tracer background concentration (M L$^{-3}$) |
| $\overline{C}$ | average solute (tracer) concentration (M L$^{-3}$) |
| $C_f$ | final tracer concentration (M L$^{-3}$) |
| $C_{i_f}$ | final measured tracer concentration corrected for background (M L$^{-3}$) |
| $C_{i_i}$ | initial measured tracer concentration uncorrected for background (M L$^{-3}$) |
| $\overline{C_i}$ | 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$^{-3}$) |
| $C\left(x_s, t\right)$ | mass of recovered tracer over distance(s), $x_s$ and time(s), $t$ [M L$^{-3}$]; |
| $D$ | 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) |
| $F$ | cumulative residence time distribution (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)

$n$    number of measured data points (dimensionless)

$n_e$    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)

$Pe$    Péclet number (dimensionless)

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

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

$r$    karst conduit radius (L)

$S_d$    sinuosity factor (dimen.)

$t$    time of sample collection (T)

$t_c$    time conversion factor (T)

$T_d$    duration in time for tracer cloud to pass any one point in the flow section (T)

$T_D$    duration in time required for entire tracer cloud to pass a flow section (T)

$T_e$    elapsed time to leading edge of tracer cloud (T)

$T_f$    elapsed time to trailing edge of tracer cloud (T)

$t_{inf}$    time tracer takes to reach the flow system (T)

$t_2$    time for tracer injection for a pulse injection (T)

$t_\kappa$    maximum allowable time for Chatwin analysis (T)

$t_p$    time to peak concentration (T)

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

$\Delta t$    time interval between multiple tracer injections (T)

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

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

$v_s$    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)

$\mathbf{x}$    vector of straight-line parameters used in the Chatwin analysis ($T^{1/2}$)

$\mathbf{x}$    vector of straight-line parameters used in the Chatwin analysis ($T^{1/2}$)

$x_s$    sinuous tracer migration distance (L)

$\delta$    laminar flow sublayer (L)

$\delta_m$    molecular diffusion layer thickness (L)

$\gamma_t$    skewness coefficient ($T^3$)

$\kappa_t$    kurtosis coefficient ($T^4$)

$\varepsilon$    relief of karst conduit wall surface irregularities (L)

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

$\pi$    pi (dimensionless)

$\rho$    fluid density (M $L^{-3}$)

$\sigma_t$    standard deviation for mean residence time (T)

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

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