# Rapid Processing of Turner Designs Model 10-AU-005 Internally Logged Fluorescence Data

Cover Figure

Flow chart for FLOWTHRU program subroutine TIMCNT explaining how FLOWTHRU handles severe time breaks in logged data files.

Rapid Processing of Turner Designs

Model 10-AU-005 Internally

Logged Fluorescence Data

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DISCLAIMER

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ABSTRACT

Continuous recording of dye fluorescence using field fluorometers at selected sampling sites facilitates acquisition of real-time dye tracing data. The Turner Designs Model 10-AU-005 field fluorometer allows for frequent fluorescence readings, data logging, and easy downloading to a laptop computer. By necessity, the data are periodically broken up into blocks to facilitate downloading and minimize data loss. Unfortunately, the downloaded data do not appear in a readily usable form for discerning trends or for use in modeling packages. A new computer program, FLOWTHRU, bypasses block headers, reads the downloaded data, identifies the time-concentration units used, and relates the data to injection time. All preinjection time-concentration data are accorded background data status and are written to a background file with average temperature values included. All time values recorded after injection time are rewritten into decimal time in time units chosen by the user. Additional features include options for processing selected percentages of the time-concentration data and for using the measured concentrations, average concentrations of data blocks, or smoothed concentrations developed using a moving average filter. FLOWTHRU also allows users to view the data converted to decimal time directly on the computer monitor without program interruption or to go directly to the data plotting routine. Data plotting is extremely rapid and clear, with a smooth line connecting each data point. Each data plot may be saved as a file in a common format.

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NOTATION

C_b Background concentration $\left[\text{M L}^{-3}\right]$

$\overline{C}_b$ Average background concentration $\left[\text{M L}^{-3}\right]$

C_p Peak concentration $\left[\text{M L}^{-3}\right]$

d Calculated number of days from time of injection

D_x Axial dispersion $\left[\text{L}^2\,\text{T}^{-1}\right]$

L Solute migration distance [L]

n Total number of time values to be recalculated to decimal time

n_b Number of background measurements

P_e Péclet number [dimen.]

Q System discharge $\left[\text{L}^3\,\text{T}^{-1}\right]$

Δs_t Time spacing for exact or even time ($1 \leq \Delta s_t \leq 10$ for Δs_t in days and $24 \leq \Delta s_t \leq 240$ for Δs_t in hours)

t Decimal time calculated from measured time using a 24-hour clock [T]

t_h Measured time in hours [h]

t_{h_r} Tracer release time hour [h]

t_{m_r} Tracer release time minutes [min]

t_m Measured time in minutes [min]

t_p Time to peak arrival [T]

t_s Measured time in seconds [s]

t_{st} Calculated tracer injection (start) time in hours [h]

t_u Multiplier to adjust decimal hours to decimal time units of choice

DESCRIPTION OF UNITS

Unit of Measure	Type of Unit	Abbreviation
	Concentration Units	
None		—
full scale units		fsu
quantitative fluorescent technique		qft
parts per million		ppm
parts per billion		ppb
parts per trillion		ppt
milligrams per liter		mg L^{-1}
milligrams per deciliter		mg dL^{-1}
grams per liter		g L^{-1}
milligrams per killigram		mg kg^{-1}
milligrams per gram		mg g^{-1}
micrograms per liter		μg L^{-1}
micrograms per milliliter		μg mL^{-1}
micrograms per kilogram		μg kg^{-1}
micrograms per gram		μg g^{-1}
nanograms per liter		ng L^{-1}
nanograms per milliliter		ng mL^{-1}
nanograms per microliter		ng μL^{-1}
nanograms per kilogram		ng kg^{-1}
nanograms per gram		ng g^{-1}
nanograms per milligram		ng mg^{-1}
picograms per gram		pg g^{-1}
picograms per milligram		pg mg^{-1}
picograms per microgram		pg μg^{-1}
picograms per milliliter		pg mL^{-1}
picograms per microliter		pg μL^{-1}
femtograms per milliliter		fg μL^{-1}
femtograms per milligram		fg mg^{-1}
relative concentration		Raw
	Mass Units	
microgram		μg

Unit of Measure	Type of Unit	Abbreviation
Time Units		
days		d
hours		h
reciprocal hours		h^{-1}
minutes		min
seconds		s
Transport Units		
meters		m
kilometers		km
meters per second		$m\ s^{-1}$
square meters per second		$m^2\ s^{-1}$
volumetric discharge		$m^3\ h^{-1}$
Temperature Units		
Celsius		°C
Fahrenheit		°F
Generic Units		
length		L
mass		M
time		T

PREFACE

The National Center for Environmental Assessment has prepared this document for the benefit of the U.S. Environmental Protection Agency regional offices, states, and the general public because of the need to develop a fast and easy method for rewriting data internally logged by a Turner Designs Model 10-AU-005 in decimal time. Application of the methodology described in this document can provide individuals with the information necessary for rapidly examining tracer test results and preparing data sets for numerical analysis.

The purpose of this document and program is to serve as a technical guide to various groups who must evaluate:

1. Travel times;

2. Dispersivities;

3. Hydraulic connections; and

4. Contributing (recharge) areas.

Tracing studies are always appropriate and probably necessary, but internally logged data are not always directly usable. This document and associated computer programs alleviate some of these problems.

The program, FLOWTHRU, allows for very rapid and easy rewriting of logged time into decimal time, prepares selected data files, and plots the data directly so that data trends may be discerned. It is believed that the use of FLOWTHRU will substantially enhance tracer test analyses.

This document and program are specific to the Turner Designs Model 10-AU-005 because it is the instrument currently used by the EPA author. EPA does not endorse this instrument or any other instrument of similar functionality. The original purpose behind the development of FLOWTHRU was to enhance data manipulation of the logged data for the equipment in use. Once developed, it was deemed sufficiently useful such that it should be placed in the public domain. Although specific to the Turner Designs Model 10-AU-005, FLOWTHRU may be easily adapted to other fluorometers with flowthrough-analysis capabilities provided a method is readily available for direct calculation of tracer dye concentrations.

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1. INTRODUCTION

Continuous data recording at selected sampling sites is widely recognized as extremely valuable for inexpensively obtaining large amounts of real-time data. Water level measurements in piezometers using pressure transducers and external data loggers are a common example of large amounts of data being logged for later analysis. Automatic fluorometric data logging of tracer dyes using field fluorometers (Turner, 1993) and external data loggers (Smart et al., 1998) are also common (Lin et al., 2003; Wilson et al., 1986, pp. 17–18).

The older Turner Model 10 Series fluorometers are still widely in use, but the Turner Designs Model 10-AU-005 benefits from a number of improvements (Smart et al., 1998). The Model 10-AU-005 field fluorometer, when fitted with a one-piece flow cell (Turner, 1993), allows fluorescence logging from every second to every 30 minutes with automatic temperature compensation included. However, the user is limited to selecting logging intervals of 1, 2, 3, 5, 10, 20, or 30 seconds or 1, 2, 3, 5, 10, 20, or 30 minutes. The total number of data points that can be logged is also limited by its memory capability (Table 1). Although a very large number of

Table 1. Internal data storage capacity of a Turner Designs Model 10-AU-005.

Logging Strategy[a]	Temperature Logging	Storage Size[b]
Cycle	With Temperature	18,510
Cycle	Without Temperature	21,600
One way	With Temperature	43,200
One way	Without Temperature	64,800

[a] Method of logging data. Cycle = Data logged chronologically until the memory is full, then old data are overwritten starting with oldest data. One way = Data logged chronologically until the memory is full, then no more data may be logged.

[b] Total number of data values that may be logged.

data values may be logged by the Model 10-AU-005, it is still fairly limited relative to an external data logger.

The Turner Designs IDL_1B1 program (Turner, 1993) provides for relatively easy downloading of data to a laptop computer, although the program currently must be run in the MSDOS mode[1]. However, by necessity, the actual logged data do not appear in a form that is amenable to data

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[1]Turner Designs has recently developed a Windows version of the IDL_1B1 program which may be obtained at http://www.turnerdesigns.com/t2/sw/main.html.

analysis and plotting. Typically, users of data downloaded from a Model 10-AU-005 must use a wordprocessor to remove block headers, edit the data, save the changes, and export the edited file into a spreadsheet program for manipulation (Turner, 1993). For large time-concentration files, this procedure can be onerous.

The purpose of this paper is to present a new computer program, FLOWTHRU, that facilitates manipulation of Model 10-AU-005 data downloaded using the IDL_1B1 program with minimal effort by the user. FLOWTHRU is not intended as a replacement for the IDL_1B1 program. Rather, FLOWTHRU provides for easy and rapid data processing and plotting of Model 10-AU-005 logged data without requiring the use of several different programs, file storage forms, or plotting software.

1.1. MODEL 10-AU-005 DATA FILE APPEARANCE

A typical logged data file downloaded from a Model 10-AU-005 fluorometer is shown in Figure 1. Several points can be made using this figure. Every logged data file begins with a Turner Designs header file that is then followed by a brief description of the fluorometer setup. The actual logged data are then listed sequentially. No column labels are provided, but the data appears as listed in Figure 1 in columns organized as:

Number   Date   Time   Concentration   Temperature   Temperature Units

where **Temperature** and **Temperature Units** do not appear if temperature logging is not set at the time of startup. The appearance of the data is relatively self-explanatory. Apparent in Figure 1 are the negative concentrations that can—and—often are recorded as a result of background fluorescence in the water sample used to "blank" or zero the fluorometer. All negative concentrations need to be converted to zero concentration, which is done by some model packages (e.g., QTRACER2). Negative concentrations may be avoided by calibrating with distilled water as a true blank then prior to any numerical analysis, reading the high blanks and subtracting them from the other readings (Turner, 1993).

1.1.1. Data Blocks

By necessity, the data file is periodically broken up into blocks to facilitate downloading. Also apparent from Figure 1 is that as new data blocks are downloaded, sample numbering begins anew for each new data block. This renumbering complicates search-and-replace operations using the sample numbers as pointers when editing the data.

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

                                         ***********************************
                                         *                                 *
                                         *   T U R N E R    D E S I G N S   *
                                         *                                 *
                                         ***********************************

                                           FLUOROMETER INTERNAL DATA LOGGER

                                                DATA OUTPUT PROGRAM

                        *******************************************************************************

                        DATA LOGGING STRATEGY:  ONE WAY


                        DATA SET NO:            1

                        DATA LOGGING METHOD:    INSTANT

                        DATA LOGGING INTERVAL:  10 (MIN)

                        DATA LOGGING UNIT:      (ug/l)

                        DATA LOGGING STARTED:   10/11/02 10:24:50
                        DATA LOGGING ENDED:     10/18/02 10:14:50

                        ===============================================================================


                        00001: 10/11/02 10:24:50 = -1.20    14.0 (C)
                        00002: 10/11/02 10:34:50 = -1.15    14.0 (C)
                           .         .        .        .        .
                           .         .        .        .        .
                           .         .        .        .        .
                        01007: 10/18/02 10:04:50 = -0.907   13.7 (C)
                        01008: 10/18/02 10:14:50 = -0.917   13.7 (C)
                        ===============================================================================

                        DATA SET NO:            2

                        DATA LOGGING METHOD:    INSTANT

                        DATA LOGGING INTERVAL:  10 (MIN)

                        DATA LOGGING UNIT:      (ug/l)

                        DATA LOGGING STARTED:   10/18/02 10:41:36
                        DATA LOGGING ENDED:     11/05/02 15:25:48

                        ===============================================================================


                        00001: 10/18/02 10:41:36 = -0.931   13.7 (C)
                        00002: 10/18/02 10:51:36 = -0.966   13.7 (C)
                           .         .        .        .        .
                           .         .        .        .        .
                           .         .        .        .        .
                        00606: 11/05/02 15:15:48 =  0.072   13.7 (C)
                        00607: 11/05/02 15:25:48 =  0.028   13.7 (C)
                        ===============================================================================
```

Figure 1. Example data file downloaded from a Turner Designs Model 10-AU-005 field fluorometer.

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Less apparent in Figure 1 is the fact that a break in the set time sequence (i.e., data-logging interval = 10 min in Figure 1) can occur during data downloading (e.g., time intervals > 10 min). This time break may occur because use of the IDL₋1B1 program requires that the Model 10-AU-005 internal logger be shut down to avoid data loss during the downloading process. However, it is possible that a scheduled sample measurement may coincide with logger shut down, causing a minor loss of data. Although the loss of one or more sample readings may not be significant, such a loss hampers the ability to perform a search-and-replace operation using measured time values as pointers when editing the data.

1.1.2. Data Interrupts

Power surges or loss of power also may result in large data interrupts, or worse, corrupted data. The only way to handle corrupted data is to erase all previously logged data and restart the logger. The newly logged data can either be treated as a stand-alone data file or they can be appended to a previously downloaded data file. In either instance, the resulting file is much more difficult to evaluate than if no data corruption had occurred.

1.1.3. Large Data Sets

Lastly, depending on the selected logging interval and the length of time that the fluorometer is run, very large data sets may be recorded. Data records $\gg$ 10,000 (but not exceeding 64,800 lines) are not unrealistic but are difficult to analyze because of the large number of data values.

1.2. DESIRED IMPROVEMENTS

To represent an improvement over the existing Model 10-AU-005 data file and the wordprocessor/spreadsheet analysis procedure, a new program should be capable of directly reading, processing, and rewriting the data file into a more useful form. All data obstructions (e.g., block headers) should be seamlessly bypassed. Manual interaction by the user should be limited to providing certain desirable aspects specified by the user.

1.2.1. Form of Data File

Although appropriate as listed, the data file shown in Figure 1 is difficult to analyze, and data trends are difficult to discern. These problem are exacerbated as the file gets larger. A more appropriate data listing would appear in decimal time starting at zero time. Such a data form facilitates data analysis by conventional numerical integration, such as is done using the computer

program, QTRACER2 (Field, 2002), or by fitting models to the data, such as with the model CXTFIT2 (Toride et al., 1995).

1.2.2. When to Start Counting

Decimal time should start at zero time, where zero time is most appropriately equated with the date and time of injection. All subsequent dates and times should then proceed sequentially. Any odd data interrupts, such as block headers and large interrupts in dates and/or times, should not prevent proper data counting and processing.

1.2.3. Data Output

The converted data should be rewritten to a data file that can be easily accessed by such common ASCII-display programs as Notepad® and Wordpad®. The file can then be copied to data input files used by other programs, such as QTRACER2 and CXTFIT2.

1.2.4. Data Plotting

Graphical plotting of the data allows trends in the data to be easily observed. This is very valuable for guiding later aspects of any particular study. The ability to save the graphical display in common file types and in vectorial and raster formats facilitates dissemination to interested parties.

2. MAIN PROGRAM DESIGN

The new program, FLOWTHRU, was developed with the intention of meeting all the previously suggested improvements. The program was written in standard FORTRAN, and the executable form can be run on any PC using Windows. It is fast, simple, and straightforward to run. Numerous subroutines included with the main program facilitate processing speed and program clarity.

2.1. MAIN PROGRAM

The main program reads all the necessary input data, processes the measured time values, and produces a file of decimal time values with corresponding concentration values suitable for use in breakthrough curve (BTC) analysis. The flowchart depicted in Figure 2 illustrates the basic flow FLOWTHRU, which is described below. For any new program such as FLOWTHRU to be a substantial improvement over other methods, it should be able to work almost seamlessly with the Model 10-AU-005 logged data file downloaded to a computer using the IDL_1B1 program. For example, when FLOWTHRU reads through the Model 10-AU-005 header information, it acknowledges whether time units were recorded in seconds (sec) or minutes (min), the time spacing for the recorded units, and the concentration units selected, which can be any one of the 28 different concentration units shown in Table 2. It will be noted from Table 2 that, whereas the Model 10-AU-005 logged data file records everything in ASCII format suitable for downloading, FLOWTHRU rewrites these into a slightly more correct scientific form.

2.1.1. Background Concentration

FLOWTHRU accepts the date and time of tracer injection, which is taken as zero time (t_1) by FLOWTHRU. All recorded time data prior to the time of injection is then accorded background status and is recorded directly to a background-data file with corresponding measured concentrations. Average background concentration $\overline{C}_b$ prior to tracer injection is added to the background data file and is obtained from

$$\overline{C}_b = \frac{1}{n_b} \sum_{i=1}^{n_b} C_{b_i} \tag{1}$$

Using the data shown in Figure 1 on page 3, FLOWTHRU produced the background data file shown in Figure 3 on page 10. Figure 3 is fairly self-explanatory in that it shows the date and time that a dye concentration was measured. At the bottom of the table depicted in Figure 3, the average background concentration is shown. This latter value is useful because the average background

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Begin Flowthru

Initialize Counters

Read Process Control File?

Y — Set Automatic Data File Processing → Read Process Control File Name → Open Process Control File → Call Data_Read

N — Set Interact. Data File Processing → Read Turner Designs Data File Name → Read New Converted Data File Name → Read New Background File Name

Open Input/ Output Files

A

Read Decimal Time Selection

A

Time = Days?

Time = Hours ?

Time = Minutes ?

Time = Seconds ?

N — A

Y

Set Decimal Time Selection

Read Turner Designs File Setup Units

View Data On Screen ?

Y — Open Tmp. File/View Control = On

N

Data Size = All ?

Data Size = Exact ?

Data Size = Even ?

Data Size = Percentage ?

N

Y

Read Time Spacing (Hours/Days)

Computer or User Chosen ?

U — Read User Percentage

C

Use Average or Measured Data ?

A

M

B

Figure 2. Flowchart depicting processing of the program FLOWTHRU.

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Figure 2. Flowchart depicting processing of the program FLOWTHRU (cont.).

Table 2. Allowable Turner Designs Model 10-AU-005 concentration units.

Model 10-AU-005 Form	FLOWTHRU Form
NONE	None[a]
FSU[b]	fsu
QFT[b]	qft
PPM	ppm
PPB	ppb
PPT	ppt
mg/l	mg L^{-1}
mg/dl	mg dL^{-1}
g/l	g L^{-1}
mg/kg	mg kg^{-1}
mg/g	mg g^{-1}
ug/l	μg L^{-1}
ug/ml	μg mL^{-1}
ug/kg	μg kg^{-1}
ug/g	μg g^{-1}
ng/l	ng L^{-1}
ng/ml	ng mL^{-1}
ng/ul	ng μL^{-1}
ng/kg	ng kg^{-1}
ng/g	ng g^{-1}
ng/mg	ng mg^{-1}
pg/g	pg g^{-1}
pg/mg	pg mg^{-1}
pg/ug	pg μg^{-1}
pg/ml	pg mL^{-1}
pg/ul	pg μL^{-1}
fg/ul	fg μL^{-1}
fg/mg	fg mg^{-1}
RAW[c]	Raw

[a] A FLOWTHRU plot will not include a display of any concentration units when the Model 10-AU-005 logged data file reads None, but the printed data tables will show "None."

[b] The Model 10-AU-005 User's Manual does not explain what these units represent. FSU represents "full scale units" which is more applicable to the old panel meter style unit; QFT represents the "quantitative fluorescence technique" that was developed by Texaco for measuring oil fluorescence in exploratory mud samples (J. McCormick, *pers. comm.*)

[c] "RAW" is not listed as one of the operational parameters in the Model 10-AU-005 User's Manual (Turner, 1993, p. A5-3), but it may be selected for calibration purposes (Turner, 1993, p. 3-10) and represents relative fluorescence. FLOWTHRU is set up to read this "unit" if it can be set as an operational parameter.

```
                    BACKGROUND CONCENTRATION
-------------------------------------------------------------
     DATE               TIME                 CONCENTRATION
                      (h)  (min)                (µg/L)
-------------------------------------------------------------
   10/11/02           10 : 24                   0.000
   10/11/02           10 : 34                   0.000
   10/11/02           10 : 44                   0.000
   10/11/02           10 : 54                   0.000
   10/11/02           11 : 04                   0.000
   10/11/02           11 : 14                   0.000
   10/11/02           11 : 24                   0.000
-------------------------------------------------------------

   AVERAGE BACKGROUND CONCENTRATION = 0.0000   µg/L
```

Figure 3. Example background data file produced by FLOWTHRU.

concentration can and should be subtracted from all measured concentrations occurring after dye injection to better represent actual sample measurements.

If the Turner Designs Model 10-AU-005 data file contains ≥5 background measurements and the average background concentration exceeds zero, then a more detailed listing of univariate statistical parameters is included at the bottom of Figure 3. The main value of this additional information (not shown in Figure 3 because the background concentration C_{b_i} did not vary) is to provide the user with a sense of the range of natural background fluorescence. The univariate statistics, developed using the equations shown in the box in Figure 4, provide a sense of the range and distribution of values potentially produced when a large number of background measurements over a relatively long period of time have been taken. Substitution of, for example, the minimum or maximum background concentration (e.g., Stat(6, ∗) and Stat(7, ∗), respectively in Figure 4) for the average background concentration may be a desirable change in some instances. A generic form of the univariate statistical output for a varying background concentration (Figure 5) was developed using data listed in the file, Break.prn (see Section 5.3.2. on page 74 for a brief discussion of Break.prn). Figure 5 illustrates the univariate statistics that would be created using the equations shown in Figure 4 .

2.1.2.   Measured Water Temperature

If water temperature was measured by a Turner Designs Model 10-AU-005 (see the last two data columns in Figure 1 on page 3) then FLOWTHRU will average the water temperature data as shown in Figure 6 on page 12. If water temperature was not measured, then a water-temperature table is still produced at the end of the background-concentration file (same file as the background-concentration table) but no water-temperature data are recorded.

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1. Mean, Stat(1, $*$)	$\overline{x}_w = \frac{\sum f_i \, w_i \, x_i}{\sum f_i \, w_i}$
2. Variance, Stat(2, $*$)	$\sigma_w^2 = \frac{\sum f_i \, w_i \, (x_i - \overline{x}_w)^2}{n-1}$
3. Standard Deviation, Stat(3, $*$)	$\sigma_w = \sqrt{\sigma_w^2}$
4. Skewness, Stat(4, $*$)	$\gamma_{x_w} = \frac{\frac{1}{n} \sum f_i \, w_i \, (x_i - \overline{x}_w)^3}{\left[\frac{1}{n} \sum f_i \, w_i \, (x_i - \overline{x}_w)^2\right]^{3/2}}$
5. Kurtosis, Stat(5, $*$)	$\kappa_{x_w} = \left\{ \frac{\frac{1}{n} \sum f_i \, w_i \, (x_i - \overline{x}_w)^4}{\left[\frac{1}{n} \sum f_i \, w_i \, (x_i - \overline{x}_w)^2\right]^2} \right\} - 3$
6. Minimum, Stat(6, $*$)	$x_{\min} = \min(x_i)$
7. Maximum, Stat(7, $*$)	$x_{\max} = \max(x_i)$
8. Range, Stat(8, $*$)	$x_r = x_{\max} - x_{\min}$
9. Coefficient of Variation, Stat(9, $*$)	$x_{cv} = \frac{\sigma_w}{\overline{x}_w} \quad$ for $\overline{x}_w \neq 0$
10. Number of values processed, Stat(10, $*$)	$n = \sum f_i$

where the statistics are given in terms of a single variable x. The i-th datum is x_i, with corresponding frequencies set to unity ($f_i = 1$) and weights also set to unity ($w_i = 1$)[a].

[a]Note that none of the variables shown in this box are intended in any way to match similar variables used elsewhere in this document. For example, x_i here represents any required input parameter (e.g., concentration, C_b) and n represents the number of measured values used to develop the mean values for each of the required parameters.

Figure 4. Equations used to calculate the univariate statistics for background concentration measurements.

```
                Univariate Statistics from UVSTA

      Mean      Variance    Std. Dev.     Skewness   Kurtosis
 0.0003235    0.2210E-06    0.0004701       0.7544    -1.4308

   Minimum     Maximum         Range    Coef. Var.      Count
    0.0000    0.001000      0.001000        1.4531   102.0000

 Lower CLM   Upper CLM     Lower CLV     Upper CLV
 0.0002312   0.0004159    0.1708E-06    0.2973E-06
```

Figure 5. Univariate statistics created for a Turner Designs data file with varying background concentrations. Note that CLM and CLV represent the confidence levels for the mean and the variance, respectively. All other table headings should be readily apparent.

```
                    AVERAGE MEASURED WATER TEMPERATURE
    -----------------------------------------------------------
    BACKGROUND WATER       SINCE INJECTION    ALL MEASURED WATER
      (°C)    (°F)           (°C)    (°F)        (°C)    (°F)
    -----------------------------------------------------------
      14.0    57.2           13.5    56.2        13.5    56.2
    -----------------------------------------------------------
```

Figure 6. Example water temperature data file produced by FLOWTHRU.

Like Figure 3, Figure 6 is fairly self-explanatory in that it shows the average background water temperature in column 1, the average water temperature from the time of dye injection in column 2, and the average water temperature for all water samples in column 3. Obviously, column 1 will be the least representative of average water temperature because it is based on the fewest water sample readings. Water temperature readings are shown in both degrees Celsius (°C) and degrees Fahrenheit (°F).

2.1.3. Decimal Time Units

The internal data logger in a Model 10-AU-005 limits data intervals to time units of seconds and minutes, which may not be the most desirable output form for very long tracer experiments (e.g., those lasting many days). FLOWTHRU allows the user to set the desired time units to decimal days, hours, minutes, or seconds (based on a 24-hour clock) regardless of what was set in the internal data logger.

This operation greatly simplifies an evaluation of a tracer test because inordinately long tracer tests may be examined with more convenient time values. Tracer experiments ≤5 hours are probably best evaluated using the time setting used to log the data (e.g., seconds or minutes). However, tracer experiments >5 hours may warrant adjusting the time setting to hours or days for a more readable output.

2.1.3.1. *Decimal Time Calculation.* Calculation of decimal time is a straightforward reworking of conventional date and time data. After subtracting out background data, FLOWTHRU reads the first date and time values that correspond with injection date and time. Using a modification of the method developed by Mull et al. (1988), the date and time values are then converted to a "start" time t_{st} (time of injection) by

$$t_{st} = \left(t_{h_1} + \frac{t_{m_1}}{60} + \frac{t_{s_i}}{3600} \right) - \left(t_{h_1} - t_{h_r} + \frac{t_{m_1}}{60} - \frac{t_{m_r}}{60} + \frac{t_{s_i}}{3600} - \frac{t_{s_r}}{3600} \right) \qquad (2)$$

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so that actual decimal time values are developed according to

$$t_i = t_u \sum_{i=1}^{n} t_{h_i} + \frac{t_{m_i}}{60} + \frac{t_{s_i}}{3600} - t_{st} + (24\, d_i) \tag{3}$$

where d is incremented by one for every instance that t_h equals 24 hours (which is reset to zero in the Turner Designs data file) in the time-concentration file and t_u adjusts t for the desired time units according to Table 3. An examination of Equations (2) and (3) shows that $t_1 = t_{st} = 0$ for the first measured time value at or immediately after the date and time of tracer release.

Table 3. Multiplier for decimal time units.

Time Units	t_u
Days	$\frac{1}{24}$
Hours	1
Minutes	60
Seconds	3600

2.1.4. Data Counting

To facilitate data processing while minimizing overhead in FLOWTHRU, the data are counted from the date and time of injection so that the necessary storage space may be dynamically allocated. The storage space is dependent on the form that the user chooses for the converted data. Processing *ALL* the data, a *PERCENTAGE* of the data, an *EXACT*-time spacing of the data, or an *EVEN*-time spacing of the data are options. If the user selects a processing option other than *ALL*, then the user may select to have the data averaged[2] and a standard deviation calculated for the concentration values, which will be displayed as error bars on the final plot, or the user may elect to have the concentration data "smoothed" using a moving average filter. Alternatively, the user may elect to just have FLOWTHRU skip to matching time-concentration data.

If just a percentage of the data is selected, then the user is given the option of having FLOWTHRU select the optimum data percentage to display. Alternatively, the user may manually select the desired data percentage, in whole numbers only, to display.

---

[2]In general, data averaging may not be considered greatly desirable because it is actually taking an average of an average. In fact, the Turner Designs Model 10-AU-005 can be specifically instructed to average concentration data for each recorded time measurement.

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Selection of exact-time or even-time spacing is allowed for daily and hourly decimal times only. An exact-time spacing is an exact listing of time readings, but data interrupts may cause uneven spacing.

Even-time spacing is a perfect spacing of time readings, but concentration values may not perfectly align with the listed times. Inconsistent listing of even-spaced times with concentration values will generally be insignificant, especially with long-term experiments and/or only minor time interruptions. This setting, however, may cause adverse effects for short-term experiments or when large time interruptions occur because insufficient data would be produced for processing. Even-time spacing should not be used when applying inverse models to the data.

2.1.5. Time Data Processing

After memory requirements have been established and the time to start data processing has been determined, FLOWTHRU enters a loop mode. It then reads in the selected time data, bypasses all time interrupts while maintaining proper time spacing, converts the time data to decimal time in the chosen units, and writes the decimal time data to a user-specified output file. If the time-concentration data are to be displayed directly on the computer monitor, FLOWTHRU then automatically calls either NOTEPAD$^{\circledR}$ or WORDPAD$^{\circledR}$, depending on file size. (More modern PCs and operating systems are capable of displaying a large amount data on screen using NOTEPAD$^{\circledR}$ only.) After processing the data, FLOWTHRU plots the data, offers the user the opportunity to have the background concentration/water temperature tables file and the decimal time-concentration data file automatically printed, and then closes out the program.

2.1.6. Data Plotting

Upon completion of time data conversion to decimal time, FLOWTHRU calls a data plotting program and correctly plots the data with the axes appropriately labeled. This file can be manually saved as a color bitmapped file (rater format) or as a Postscript file (vector format) in either black-and-white or color formats. Color PostScript files can have either a light blue background or a black background.

2.1.6.1. *PostScript File Descriptions.* Three Postscript file formats are provided in FLOWTHRU in order to meet selected presentation demands by the user. For typical document presentation, a simple black-and-white display may be desirable in most instances because there is no competing information (e.g., multiple data displays) on the plot that could cause confusion, memory require-

ments are smaller, and there is no need to access a color printer. In other circumstances, a color PostScript plot may be desirable.

In some instances, a presentation may benefit from a color plot. The user may select a color plot with a light blue background, black labels, purple data points, and a red line connecting the data points. Alternatively, in some instances the user may prefer to display a color plot with a black background (e.g., a slide presentation), which will have yellow labels, cyan data points, a red line connecting the data points, and a purple key indicating the number of data values processed. Figure 7 on the next page shows the three different formats developed by FLOWTHRU using the Turner Designs data referenced in Table 1 on page 3. In Figure 7 the black background color plot appears to be the least clear of the three, but this is a consequence of producing the plot at a reduced size and displaying it in a printed document. The main purpose of producing a color PostScript plot with a black background would be for slide presentations, in which case the plot will be much clearer.

As shown in Figure 7, each plot has a key, shown in the upper right-hand corner, that indicates the number of data points and the percentage of the total number of data points processed. The plots indicate that 143 data values were processed (`Data = 143`), which has little meaning to anyone unfamiliar with the true data size (19,995 data points); the indication that only 0.72% (`Perc = 0.72%`) of the data are displayed is a pretty clear indication that only a small fraction of the data were processed for these figures. Such a small percentage was chosen in this instance because it was desirable that the display not be overwhelmed by an excessive amount of data. In addition, a computer-determined *PERCENT* of the data (see Section 2.1.4.) was chosen for the desired data-processing mode, which caused FLOWTHRU to automatically determine that only 143 data values would be processed in this instance.

2.1.7. Memory Usage

For most of the program operation, converted data are written directly to an output file. In those instances in which the user desires to examine the data directly on screen using either NOTEPAD® or WORDPAD®, the data are written to a temporary file that is deleted after closing NOTEPAD® or WORDPAD®. Array storage is necessary, however, for passing the converted data to the plotting routine, so only two or three storage arrays are required.

In all instances, two arrays are always required: one for decimal time and one for measured tracer concentration. For those instances in which averaged or smoothed concentration values are requested, then a third array is required for the display of error bars representing the standard deviation for each average concentration (confidence limits around smoothed concentra-
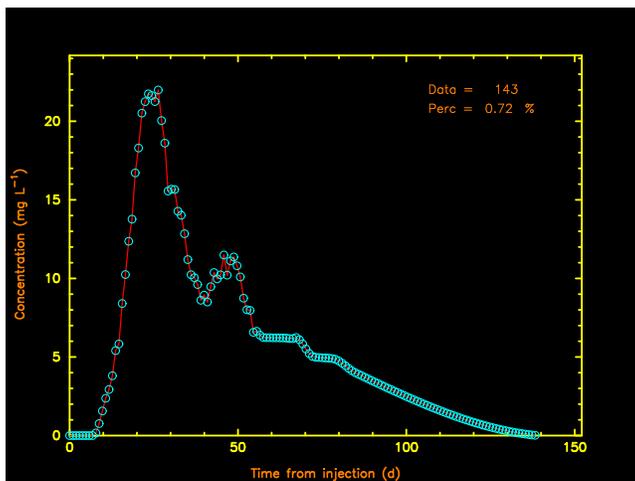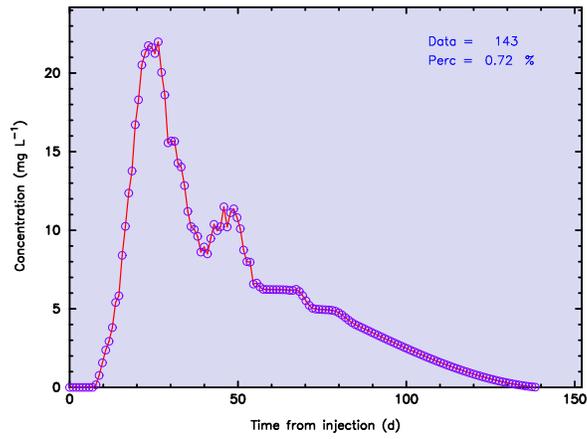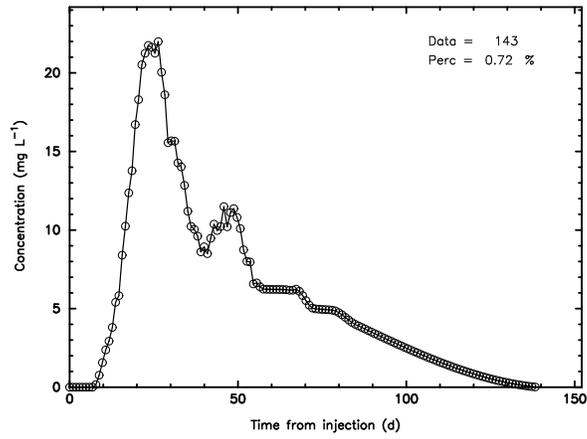
Figure 7. Three PostScript formats produced by FLOWTHRU using the Turner Designs data referenced in Table 1.

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tions). Standard-deviation values are shown when on-screen display using either NOTEPAD® or WORDPAD® is requested but are not written to the output file. Standard-deviation values and/or confidence limits are not written to the output file because such an additional column of data would not conform with typical file input requirements of breakthrough-curve analysis programs.

2.1.7.1. *Dynamic Memory Allocation.* To further minimize excess memory usage, FLOWTHRU carefully counts through the Turner Designs data file from the time of tracer injection t_1 to calculate the maximum amount of space required. The memory size is then further optimized by adjusting the maximum necessary amount downwards as appropriate for a user selection of a reduced data set (e.g., percentage, exact-time data spacing, or even-time data spacing) for conversion (see Section 2.1.4. on page 13).

In addition, when a reduced data set of either exact-time or even-time data spacing is requested, FLOWTHRU will recalculate the required memory size according to time, relative to whether the original data were measured in units of seconds or minutes. Although it may be argued that this additional recalculation is unnecessary, inclusion of this option facilitates PC multitasking, which allows a user to utilize other related programs while processing the data.

3. PROGRAM SUBROUTINES

To improve program readability and decrease processing time, several subroutines have been included in FLOWTHRU. The subroutines also effectively reduced the number of programming lines for repeated operations (e.g., DTRWND; see Section 3.2.1. on page 32). Of the subroutines included in FLOWTHRU, only the process control subroutine, FILE_PROC, is described in detail because it allows for considerable interaction by the program user. All other subroutines are described only briefly.

3.1. INTERPROCESS CONTROL SUBROUTINE

The original development of FLOWTHRU required that the user respond interactively to queries presented by FLOWTHRU. Although this option still exists in the final version, an easier option is now provided in the form of an interprocess control file, which essentially contains all the necessary control statements required by FLOWTHRU so that the program runs quickly without any additional user input. The form of the subroutine used to read and process this file is depicted in Figure 8.

The format of an interprocess control file is fairly short and easy to understand. A comment line precedes each required data line so that the user has a reminder of what the data line should contain. Figure 9 illustrates the general form of a typical flowing stream input file, the components of which are briefly described in Table 4. Note that the *Line* numbers listed in Figure 9 correspond to the *Line* numbers listed in Table 4. No column numbers are provided because *free format* input is permitted (i.e., the placement of input items is mostly irrelevant). It is apparent that all odd-numbered lines listed in Figure 9 and Table 4 are just comment lines and can contain anything that the user decides should appear on such a line or they can be left "blank." However, in no instance can one of these lines be removed from the process control file. In addition, *Line* 2 is also a comment line, as are any lines that appear after *Line* 28.

It should also be apparent from Figure 9 that the odd-numbered lines running from *Line* 9 to *Line* 27 list the options that may be recorded on the following line. Such included information helps prevent incorrect entries on the line following the listed comment line. However, FLOWTHRU specifically checks for incorrect entries, attempts to correct these entries, and then continues processing the data[3].

---

[3]Note that *all* 28 lines must appear in the interprocess control file or program operation will be terminated (this is the only instance where FLOWTHRU is programmed to terminate because of incorrect file entry). However, any number of lines greater than 28 may appear in the process control file, but *Line* 29 and subsequent lines will all be treated as comments to be ignored by FLOWTHRU.
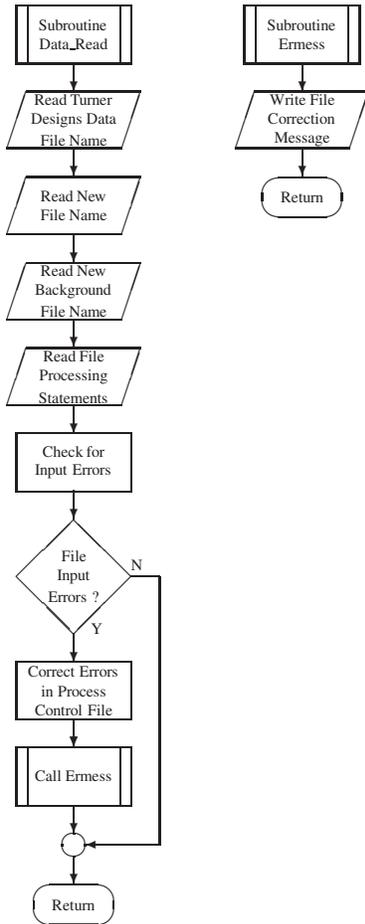
Figure 8. Flowchart depicting subroutine for implementing interprocess control file and error reporting.

Line	Generic Interprocess-Control Input File

```
1     DATA FILE FOR CONTROLLING DEFAULT INPUT FILE
2     ******************************************************************
3     FILE NAME FOR TURNER DESIGNS CREATED DATA FILE
4     Turner Designs Data File
5     FILE NAME FOR FILE OF CONVERTED TIME-CONCENTRATION DATA
6     Decimal time-concentration Data File
7     FILE NAME OF BACKGROUND DATA AND AVERAGE TEMPERATURES
8     Background Data File
9     PREFERRED TIME UNITS FOR DATA PROCESSING ([D]ay, [H]our, [M]inutes, [S]econds, [A]ll)
10    Day
11    CONTROL FOR DETERMINING IF DATA ARE TO BE DISPLAYED ON SCREEN ([Y]es/[N]o)
12    Yes
13    DESIRED FORM OF THE DATA TO BE PROCESSED ([A]ll, [P]ercent, [E]xact, e[V]en)
14    All
15    NUMBER OF DAYS OR HOURS FOR EXACT OR EVEN SPACING (1<=Day<=10, 24<=Hour<=240)
16    1
17    CONTROL FOR COMPUTER SELECTED OR USER SELECTED PERCENT DETERMINATION ([C]omputer/[U]ser)
18    Computer
19    READ USER-SELECTED PERCENTAGE AS APPROPRIATE (1 <= % <= 100)
20    10
21    CONTROL FOR MATCHING, SMOOTHING, OR AVERAGING DATA ([M]atch/[S]mooth/[A]verage)
22    Match
23    DATE AND TIME OF TRACER INJECTION (MM/DD/YY HH MN)
24    10/11/02 1025
25    POSTSCRIPT FILE CREATION CONTROL ([Y]es/[N]o)
26    Yes
27    FORM OF POSTSCRIPT FILE TO BE CREATED (0, 1, 2, 3)
28    2
29    ******************************************************************
30    STOP PROCESSING
31    END OF RUNS
```

Figure 9. Generic example of interprocess control input file illustrating the basic format used by FLOWTHRU for processing. Note that the *Line* numbers are not part of a typical input file and are listed here only for reference purposes for Table 4.

Table 4. Description of the input file components listed in Figure 9.

Line	Type	Identifier	Description
1	$\cdots$	$\cdots$	Comment line.
2	$\cdots$	$\cdots$	Comment line.
3	$\cdots$	$\cdots$	Comment line.
4	Character	FILE NAME	Turner Designs data file. This is just the actual name of the data file that is downloaded from a Model 10-AU-005 using the program, IDL_1B1.
5	$\cdots$	$\cdots$	Comment line.
6	Character	FILE NAME	Converted time-concentration file name. This is a user-chosen file name where the newly created decimal time-concentration data are to be recorded.
7	$\cdots$	$\cdots$	Comment line.
8	Character	FILE NAME	Background data file name. This is a user-chosen file name for recording the background time-concentration data and the measured temperature data.
9	$\cdots$	$\cdots$	Comment line.
10	Character	TIME UNITS	Desired time units to be used when calculating decimal time ([D]ay, [H]our, [M]inutes, [S]econds, [A]ll).
11	$\cdots$	$\cdots$	Comment line.
12	Character	SWITCH	Control switch that allows the user to view the converted (decimal) time-concentration data on the computer monitor if desired.
13	$\cdots$	$\cdots$	Comment line.
14.	Character	FORM	Form of the data for the converted (decimal) time-concentration data file. (Exact and even options ignored if *Line* 10 equals [M]inutes, [S]econds, or [A]ll.)
15	$\cdots$	$\cdots$	Comment line.

Table 4. Description of the input file components (*continued*).

Line	Type	Identifier	Description
16	Integer	SPACING	User-selected number of days ($1 \leq \Delta s_{t_d} \leq 10$) or hours ($24 \leq \Delta s_{t_h} \leq 240$) to be used when exact- or even-time spacing is desired. (Ignored if **Line 10** equals [M]inutes, [S]econds, or [A]ll.)
17	⋯	⋯	Comment line.
18	Character	SWITCH	Control switch for allowing FLOWTHRU to determine the "optimal" percentage of data to process or to allow the user to select a desired percentage to process.
19	⋯	⋯	Comment line.
20	Integer	PERC.	User-selected percentage of data to process — only whole numbers allowed. (Ignored if **Line 18** equals Computer or **Line 14** does not equal Percent.)
21	⋯	⋯	Comment line.
22	Character	SWITCH	Control switch for selecting measured concentration data, smoothed concentrations, or averaged concentrations. (In most instances the user will want to select, [M]atch; less often, [S]mooth; and rarely [A]verage.)
23	⋯	⋯	Comment line.
24	Character	INJECTION	Date and time of tracer injection in the form of MM/DD/YY HH MN SS, or MM DD YY HHMN SS. (Note that time may appear as either HH MN SS or HHMN SS.)
25	⋯	⋯	Comment line.
26	Character	SWITCH	Control switch that allows the user to have a PostScript plot file created if desired.
27	⋯	⋯	Comment line.
28	Integer	PostScript	User-choice for determining form of PostScript file to be created. (Ignored if **Line 26** equals [N]o)

Table 4. Description of the input file components (*continued*).

Line	Type	Identifier	Description
29	$\cdots$	$\cdots$	Comment line.
30	$\cdots$	$\cdots$	Comment line.
31	$\cdots$	$\cdots$	Comment line.
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

3.1.1. Line-by-Line Description of Input Files

Figure 9 and Table 4 include a ***Line*** number to identify the line on which a particular item must be supplied in a data input file. These ***Line*** numbers are provided here only as a guide to the user and are never to be included in any actual data input file. Below is a detailed description of each line for a typical data input file.

***Lines* 1 and 2** are comment statements provided for the user to enter clarifying statements that are ignored by FLOWTHRU. These lines are generally used as a convenient identifier and input file line break, both of which have no meaning.

***Line* 3** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line* 4**, which is READ by the program. For example, Figure 9 lists ***Line* 3** as:

```
FILE NAME FOR TURNER DESIGNS CREATED DATA FILE
```

which is stating that ***Line* 4** is a file name to be READ by FLOWTHRU. ***Line* 3** can be left blank if desired.

***Line* 4** is a required *user-supplied file name* (e.g., Turner Designs Data File) to be READ by FLOWTHRU. It is intended to be an identifier for the specific tracer test data being collected. For example, Figure 9 lists ***Line* 4** as:

Turner Designs Data File

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which should match all references to the actual data file. A default name is given as: `Fluor_time.prn`.

Line 5 is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line 6***, which is READ by the program. For example, Figure 9 lists ***Line 5*** as:

`FILE NAME FOR FILE OF CONVERTED TIME-CONCENTRATION DATA`

which is stating that ***Line 6*** is a file name to be READ by FLOWTHRU. ***Line 5*** can be left blank if desired.

Line 6 is a required *user-supplied file name* to be READ by FLOWTHRU. It is intended to be the name of the file that all the newly created decimal time-concentration data get written to by FLOWTHRU. For example, Figure 9 lists ***Line 6*** as:

Decimal time-concentration Data File

A default name is given as: `Fluor_time.cnv`.

Line 7 is a comment statement provided to the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line 8***, which is READ by the program. For example, Figure 9 lists ***Line 7*** as:

`FILE NAME OF BACKGROUND DATA AND AVERAGE TEMPERATURES`

which is stating that ***Line 8*** is a file name to be READ by FLOWTHRU. ***Line 7*** can be left blank if desired.

Line 8 is a required *user-supplied file name* to be READ by FLOWTHRU. It is intended to be the name of the file that all the background time-concentration data and temperature data get written to by FLOWTHRU. For example, Figure 9 lists ***Line 8*** as:

Background Data File

A default name is given as: `Fluor_time.bak`.

Line 9 is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line 10***, which is READ by the

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program. For example, Figure 9 lists *Line* **9** as:

```
PREFERRED TIME UNITS FOR DATA PROCESSING ([D]ay, [H]our, [M]inutes, [S]econds, [A]ll)
```

which is stating that *Line* **10** is a data item to be READ by FLOWTHRU. *Line* **9** can be left blank if desired.

Line **10** is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* **9** above (and in Figure 9 and Table 4), *Line* **10** can be either [D]ay, [H]our, [M]inutes, [S]econds, or [A]ll[4]. However, the items to be listed on *Line* **10** can also appear as D, H, M, S, or A in upper or lower case letters because only the first letter entered anywhere on *Line* **10** is actually READ by FLOWTHRU. For example, Figure 9 lists *Line* **10** as:

```
Day
```

which means that time-data processing by FLOWTHRU should be in decimal days.

Line **11** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* **12**, which is READ by the program. For example, Figure 9 lists *Line* **11** as:

```
CONTROL FOR DETERMINING IF DATA ARE TO BE DISPLAYED ON SCREEN ([Y]es/[N]o)
```

which is stating that *Line* **12** is a data item to be READ by FLOWTHRU. *Line* **11** can be left blank if desired.

Line **12** is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* **11** above (and in Figure 9 and Table 4), *Line* **12** must appear as either Yes[Y] or No[N] anywhere on *Line* **12** (case does not matter). For example, Figure 9 lists *Line* **12** as:

```
Yes
```

which means that, after processing by FLOWTHRU, the new time-concentration data file

---

[4]Note [A]ll here only means that data processing will be in Seconds and the x-axis of the plot will be in days, hours, minutes, and/or decimal seconds (DD HH MM SS.S) as exponents as appropriate (e.g. 10 days, 2 hours, 35 minutes, and 12.4 seconds could appear as $10^d 2^h 35^m 12.4^s$). In most instances, just a single time unit (e.g., 10^d) will appear under each major tick on the x-axis.

should be printed to the computer monitor using either NOTEPAD® or WORDPAD®.

***Line* 13** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line* 14**, which is READ by the program. For example, Figure 9 lists ***Line* 13** as:

```
DESIRED FORM OF THE DATA TO BE PROCESSED ([A]ll, [P]ercent, [E]xact, e[V]en)
```

which is stating that ***Line* 14** is a data item to be READ by FLOWTHRU. ***Line* 13** can be left blank if desired.

***Line* 14** is a required data entry item to be READ by FLOWTHRU. As indicated by ***Line* 13** above (and in Figure 9 and Table 4), ***Line* 14** must appear as All[A], Percent[P], Exact[E], or Even[V] anywhere on ***Line* 14** (case does not matter). For example, Figure 9 lists ***Line* 14** as:

```
All
```

which means that all the measured time-concentration data are to be processed by FLOWTHRU.

***Line* 15** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for ***Line* 16**, which is READ by the program. For example, Figure 9 lists ***Line* 15** as:

```
NUMBER OF DAYS OR HOURS FOR EXACT OR EVEN SPACING (1<=Day<=10, 24<=Hour<=240)
```

which is stating that ***Line* 16** is a data item to be READ by FLOWTHRU. ***Line* 15** can be left blank if desired.

***Line* 16** is a required data entry item to be READ by FLOWTHRU. As indicated by ***Line* 15** above (and in Figure 9 and Table 4), ***Line* 16** must appear as a numerical value ranging from 1 to 10 for spacing in days or as a numerical value ranging from 24 to 240 for spacing in hours anywhere on ***Line* 16**[5]. For example, Figure 9 lists ***Line* 16** as:

```
1
```

---

[5]***Line* 16** is ignored when ***Line* 10** does not equal Day[D] or Hour[H].

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which means that all the measured time-concentration data are to be processed by FLOWTHRU on a single daily basis.

Line **17** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* **18**, which is READ by the program. For example, Figure 9 lists *Line* **17** as:

```
CONTROL FOR COMPUTER SELECTED OR USER SELECTED PERCENT DETERMINATION ([C]omputer/[U]ser)
```

which is stating that *Line* **18** is a data item to be READ by FLOWTHRU. *Line* **17** can be left blank if desired.

Line **18** is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* **17** above (and in Figure 9 and Table 4), *Line* **18** must appear as either Computer[C] or User[U] anywhere on *Line* **18**[6] (case does not matter). For example, Figure 9 lists *Line* **18** as:

```
Computer
```

which means that if a percentage of the data is to be processed by FLOWTHRU, then FLOWTHRU is tasked with determining the "optimum" percentage of data to process.

Line **19** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* **20**, which is READ by the program. For example, Figure 9 lists *Line* **19** as:

```
READ USER-SELECTED PERCENTAGE AS APPROPRIATE (1 <= % <= 100)
```

which is stating that *Line* **20** is a data item to be READ by FLOWTHRU. *Line* **19** can be left blank if desired.

Line **20** is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* **19** above (and in Figure 9 and Table 4), *Line* **20** must appear as a numerical value ranging from 1 to 100 (in whole numbers only) anywhere on *Line* **20**[7]. For example, Figure 9 lists *Line* **20** as:

---

[6]*Line* **18** is ignored when *Line* **14** does not equal Percent.
[7]*Line* **20** is ignored when *Line* **14** does not equal Percent[P] and/or *Line* **18** does not equal User[U].

which means that only 10% of the measured time-concentration data are to be processed by FLOWTHRU if allowed by *Lines* **14** and **18**.

Line **21** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* **22**, which is READ by the program. For example, Figure 9 lists *Line* **21** as:

```
CONTROL FOR AVERAGING TIME DATA OR MATCHING TIMES ([M]atch/[S]mooth/[A]verage)
```

which is stating that *Line* **22** is a data item to be READ by FLOWTHRU. *Line* **21** can be left blank if desired.

Line **22** is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* **21** above (and in Figure 9 and Table 4), *Line* **22** must appear as either Match[M], Smooth[S], or Average[A] anywhere on *Line* **22** (case does not matter). The parameter Match[M] tells FLOWTHRU to use matching measured concentrations, parameter Smooth[S] tells FLOWTHRU to use a moving average to smooth the measured concentrations, and parameter Average[A] tells FLOWTHRU to average the measured concentrations. For example, Figure 9 lists *Line* **22** as:

```
Match
```

which means that, of the time data to be processed by FLOWTHRU, the measured concentration data are to be used.

Line **23** is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* **24**, which is READ by the program. For example, Figure 9 lists *Line* **23** as:

```
DATE AND TIME OF TRACER INJECTION (MM/DD/YY HH MN SS)
```

which is stating that *Line* **24** is a data item to be READ by FLOWTHRU. *Line* **23** can be left blank if desired.

Line 24 is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* 23 above (and in Figure 9 and Table 4), *Line* 24 must appear with a date and time of injection anywhere on *Line* 24. (NOTE: Seconds, SS, need not be entered.) For example, Figure 9 lists *Line* 24 as:

```
10/12/02 1025
```

which is the date and time of tracer injection.

Line 25 is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* 26, which is READ by the program. For example, Figure 9 lists *Line* 25 as:

```
POSTSCRIPT FILE CREATION CONTROL ([Y]es/[N]o)
```

which is stating that *Line* 26 is a data item to be READ by FLOWTHRU. *Line* 25 can be left blank if desired.

Line 26 is a required data entry item to be READ by FLOWTHRU. As indicated by *Line* 25 above (and in Figure 9 and Table 4), *Line* 26 must appear as either Yes [Y] or No [N] anywhere on *Line* 26 (case does not matter). For example, Figure 9 lists *Line* 26 as:

```
Yes
```

which means that after processing by FLOWTHRU, a PostScript time-concentration data plot file should be created.

Line 27 is a comment statement provided for the user to enter a clarifying statement that is ignored by FLOWTHRU. It is generally used as a convenient label for *Line* 28, which is READ by the program. For example, Figure 9 lists *Line* 27 as:

```
FORM OF POSTSCRIPT FILE TO BE CREATED (0, 1, 2, 3)
```

which is stating that *Line* 28 is a data item to be READ by FLOWTHRU. *Line* 27 can be left blank if desired.

Line* 28** is a required data entry item to be READ by FLOWTHRU. As indicated by ***Line* 27** above (and in Figure 9 and Table 4), ***Line* 28** must appear as either 0, 1, 2, or 3 anywhere on ***Line* 28[8]*. Option 0 means no PostScript file is created — ***Line* 28** is overridden if Yes[Y] is listed on ***Line* 28***. Option 1 means that a black-and-white PostScript file is to be created if a Yes[Y] occurs on ***Line* 28**. Option 2 means that a color PostScript file with a light blue background is to be created if a Yes[Y] occurs on ***Line* 28**. Option 3 means that a color PostScript file with a black background is to be created if a Yes occurs on ***Line* 28**. For example, Figure 9 lists ***Line* 26** as:

```
2
```

which means that after processing by FLOWTHRU, a color PostScript time-concentration data plot file with a light blue background (see Section 2.1.6. and Figure 7) should be created.

3.2. ARRAY-SIZE ALLOCATION ADJUSTMENT SUBROUTINE

In order to minimize memory requirements, FLOWTHRU specifically allocates the amount of memory required. The program determines the necessary array sizes to allocate for those instances for all the data or for those instances where only a portion of the measured time-concentration data are to be processed (e.g., Percentage). This allows FLOWTHRU to use less memory, which is mostly an issue for older computers but is still a concern in some instances. To allocate an appropriate memory size, FLOWTHRU first determines what time spacing and time units were used to log the data, as listed in the header information in the Turner Designs data file (see Figure 1 on page 3). Then depending on whether time was recorded in seconds or minutes and if only a portion of the data is to be processed, FLOWTHRU calls either subroutine SUNIT or subroutine MUNIT to adjust memory allocation. Memory size is adjusted down from a full count of all data recorded according to the time spacing and units used to log the data. The subroutine flow for subroutine SUNIT is described in Figure 10.

The values N4 and N7 shown in Figure 10 are used by FLOWTHRU to adjust memory allocation. For time units recorded in minutes, subroutine MUNIT appears similar to SUNIT, but all values listed for N4 are reduced by a factor of 60. For those instances when decimal time is to be in units other than days (e.g., hours), the calculated value for N4 is increased by adding the

---

[8]Ignored if No[N] appears on ***Line* 26**.
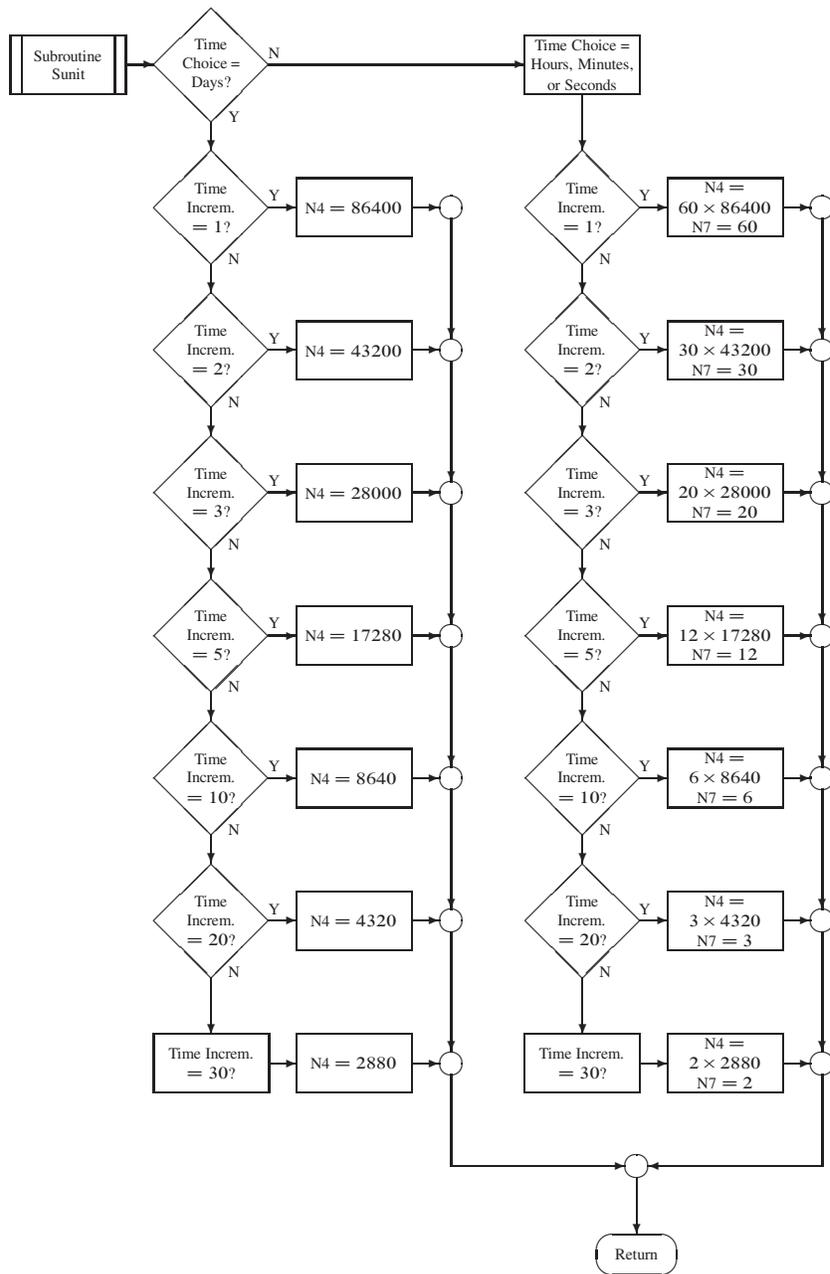
Figure 10. Flowchart depicting subroutine for memory size determination based on seconds.

value for N7.

3.2.1. Data-Counting Control

After determining if memory requirements are to be reduced from the maximum, the measured time-concentration data are counted while by-passing the initial Turner Designs data file header information and all data block separators. The header separator blocks are by-passed by use of subroutine DTRWND the flow of which is described in Figure 11.
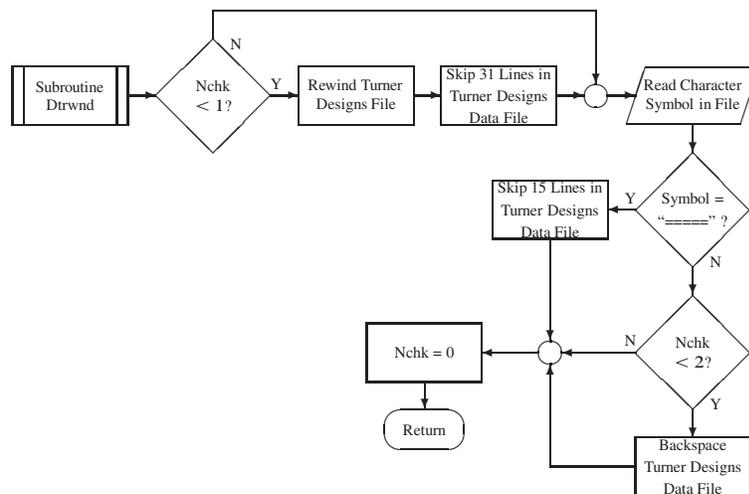
Figure 11. Flowchart depicting subroutine for counting past Turner Designs header and separate data blocks.

3.2.2. Data Time Breaks

After calling DTRWND to adjust data counting, FLOWTHRU compares the listed date and time values with the date and time of injection so that background may be properly established. If odd and/or long time breaks occur in the data (as occur when the logger is shut down for data downloading or when a power outage occurs), then FLOWTHRU calls the subroutine TIMCNT. Subroutine TIMCNT reads through the time break and apportions the necessary missing time to the decimal time-concentration data file so that an accurate passage of time may be provided. See Figure 12 for a flowchart illustrating the process used by TIMCNT.

3.2.2.1. *Leap Year Calculation.* In some instances, data time breaks may cross into and beyond the month of February, which, rarely, has 29 calendar days as a result of a leap year.
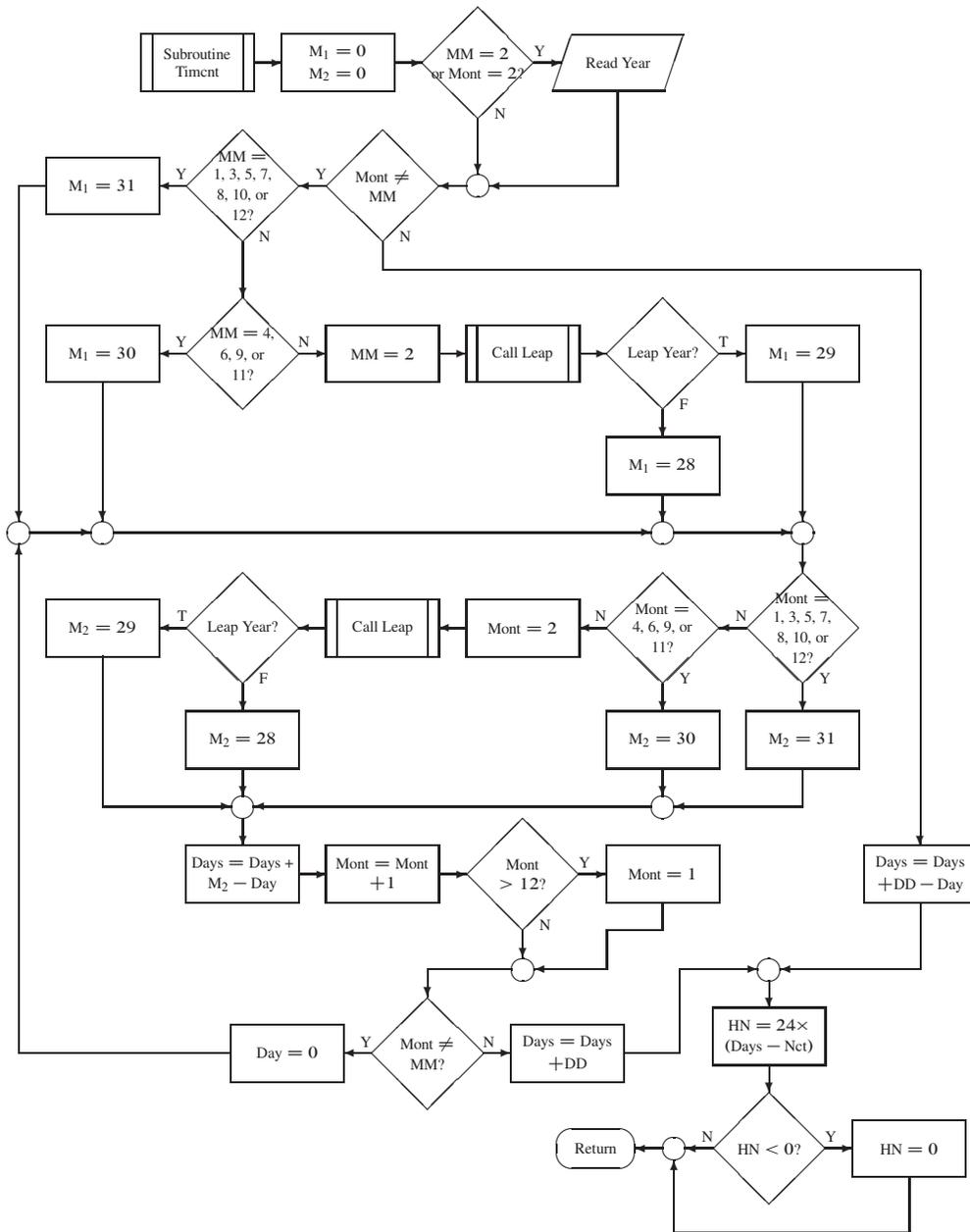
Figure 12. Flowchart depicting subroutine for counting past time breaks in the Turner Designs data file.
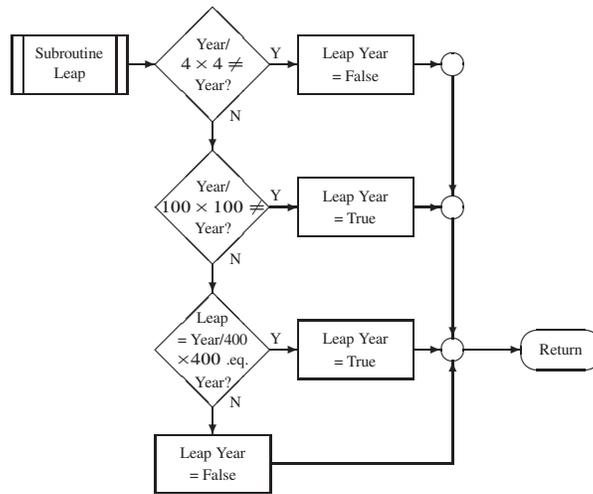
Figure 13. Flowchart depicting subroutine for determining whether time breaks in the data occurred in February during a leap year.

Subroutine LEAP (Figure 13), accessed by subroutine TIMCNT, determines whether the given year is a leap year. Figure 13 illustrates how subroutine LEAP determines whether the year is a leap year according to the following rules:

Rule 1. Every year exactly divisible by 4 is a leap year (1996 was a leap year).

Rule 2. Except those years exactly divisible by 100 are not leap years (1900 was not a leap year).

Rule 3. Except those years exactly divisible by 400 are leap years (2000 was a leap year).

Subroutine LEAP properly implements all of these rules correctly. Many current spreadsheet programs follow only rules 1 and 2, but not 3, so they treat the year 2000 as a "common year" rather than as a leap year. (The existence of "corrective macros" have actually prevented the underlying bug from being fixed.) Many other programs use only rule 1, so that they incorrectly consider the year 1900 to be a leap year, even though they get the year 2000 right, by accident (ACCC, 1998).

Subroutine LEAP was implemented in FLOWTHRU by utilizing the FORTRAN requirement of conducting operations on integers by integers (whole numbers). For example, when the year 2000 is divided by 4, the result is 500 (in whole numbers), which when multiplied by 4 returns 2000. The actual determination that the year 2000 is a leap year by subroutine LEAP is as follows:

1. $2000/4 = 500$

   $500 \times 4 = 2000$ [$2000 = 2000 \rightarrow$True]   Go to 2

2. $2000/100 = 20$

   $20 \times 100 = 2000$ [$2000 = 2000 \rightarrow$True]   Go to 3

3. $2000/400 = 5$

   $5 \times 400 = 2000$ [$2000 = 2000 \rightarrow$True]$^{\checkmark}$ Year 2000 is a leap year!

However, when the year 2006 is divided by 4, the result is 501 (in whole numbers), which when multiplied by 4 returns 2004 rather than 2006. The actual determination that the year 2006 is not a leap year by subroutine LEAP is as follows:

1. $2006/4 = 501$

   $501 \times 4 = 2004$ [$2004 \neq 2006 \rightarrow$False]$^{\checkmark}$ Year 2006 is not a leap year!

Although subroutine LEAP should be implemented only rarely, it is appropriate that it be done correctly. The need to accurately calculate solute travel times cannot be overstated.

3.3.   DECIMAL TIME FILE AND PLOT FILE HEADERS

To ensure that the results of FLOWTHRU are properly labeled so that confusion regarding time and concentration units are avoided, FLOWTHRU examines the Turner Designs data file header for the units originally set when the logger was switched on. Although there are only two different time units that FLOWTHRU needs to consider (minutes and seconds are the only time units allowed by the Turner Designs Model 10-AU-005 data logger), there are 28 concentration units that FLOWTHRU needs to recognize.

Subroutine BUNIT simply takes the listed concentration units and stores the relevant components in appropriate variables, which are then used in the plotting routine for y-axis labeling. Subroutine CUNIT performs the same basic function as BUNIT except that it instead writes a concentration header to the converted decimal time-concentration data file.

3.4.   TIME-CONCENTRATION DATA AVERAGING

As mentioned in Section 2.1.4. on page 13, time-concentration data averaging should generally not be done. However, if the user would like to have a set of concentration values averaged up to a specific time, then the subroutine AVECNT will add the required number of concentration values and their squared values. Then subroutine AVESTN will solve for the mean concentration and

standard deviation, the values of which are recorded as vectors using subroutine ARRAYS. Lastly, subroutine RESET is called to reset all variables back to zero and to begin the process over.

3.5. MEAN TEMPERATURE CALCULATION

As described in Section 2.1.2. on page 10, FLOWTHRU produces a listing of the mean water temperature recorded during the tracer test. The mean water temperatures are appropriately calculated after data processing by FLOWTHRU has been completed and the information passed to subroutine TEMPER. The mean temperature values are then converted to either degrees Celsius (°C) or degrees Fahrenheit (°F) depending on the units originally set by the user.

4. USING FLOWTHRU TO EVALUATE MODEL 10-AU-005 DATA

FLOWTHRU is an easy-to-use package that is intended to provide the user with a quick conversion of the Model 10-AU-005 logged data to decimal time with a plot of the BTC so that trends in the data may be observed. Data processing may occur by reading in an "interprocess-control file" (described in Section 3.1.) or interactively. Input errors are corrected automatically by FLOWTHRU with a screen notice to the user so that processing may proceed uninterrupted.

4.1. FLOWTHRU PROGRAM USAGE AND EXAMPLE DATA FILES

NOTE: This program functions best with a display equal to 1024×768 pixels, adequately with a display equal to 800×600 pixels, and not so well with further reduced display settings.

Before running the program, all FLOWTHRU files should be copied to the PC's hard drive. Although plenty of storage space is available on the CD-ROM disk for the creation of data output files and graphics files, the possibility of damage to the FLOWTHRU program file from excess use cannot be ignored.

4.1.1. Loading FLOWTHRU and Example Data Files

1. After booting up the computer, place the CD-ROM disk into the computer's CD-ROM disk 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 hit the letter "E" on the keyboard.

4. Place the mouse pointer on the CD-ROM disk 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 hit 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 *Left Click* on "Copy" or just hit "C" on the keyboard.

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

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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 *Left Click* on "Paste" or just hit "P" on the keyboard.

A folder named FLOWTHRU will be created on the chosen hard drive and all the appropriate files copied accordingly to the appropriate file folders[9].

4.2. FLOWTHRU EXECUTION

FLOWTHRU is very easy to use. After the appropriate data files are created (which are nearly self-explanatory), FLOWTHRU, for the most part, requires nothing more than hitting <Enter> as requested or manipulating the mouse and clicking with the left mouse button. (See Section 3.1. on page 18 for a detailed discussion of FLOWTHRU data input files.)

1. In Windows Explorer, *Left Double-Click* the FLOWTHRU folder and then *Left Double-Click* the FLOWTHRU.EXE file to initiate program operation.[10]

2. At this point, FLOWTHRU will open the program initiation screen and title (Figure 14) and will prompt the user to press <Enter> to begin full program interaction. Next, the user is requested to enter an input file name for the file to be evaluated. One advantage of a subdirectory on the hard disk is that providing an obscure path for all subfiles is not required; the program will find them automatically because they are all at the same location as the executable file. If the data files are in different locations from FLOWTHRU, the correct path to the *.inp files must be provided. Alternatively, pressing <Enter> will automatically cause FLOWTHRU to bypass usage of an interprocess control file (e.g., *.inp or any file name representing a file of the form depicted in Figure 9) and go directly into the interactive mode.

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[9]FLOWTHRU was not designed for MSDOS®use, which requires that the files be moved according to the following instructions:

- At the C:\> prompt, type "MKDIR FLOWTHRU" (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 Flowthru_dos on the CD to the hard disk (e.g., if C is the disk drive: "COPY D:*.* C:\FLOWTHRU*.*").
- Repeat the above commands for the other files on the CD.
- Put the CD in a safe location.

[10]If a command prompt is preferred, then at the C:\> prompt type "CD\FLOWTHRU" without the quotes. The user will then see a new prompt; C:\FLOWTHRU>. The user may now type "FLOWTHRU" to run the program by just responding to the requested information, assuming that the user has also copied, as created, the necessary data files.

```
*****************************************************************
*                                                               *
*                        FLOWTHRU.EXE                           *
*                                                               *
*     PROGRAM TO CONVERT TURNER DESIGNS MODEL 10-AU-005         *
*        SAMPLE TIME DATA TO DECIMAL TIME DATA FOR USE          *
*          WITH QTRACER2 AND OTHER MODELING PACKAGES            *
*                                                               *
*                         DEVELOPED                             *
*                                                               *
*                            BY                                 *
*                                                               *
*                     MALCOLM S. FIELD                          *
*            U.S. ENVIRONMENTAL PROTECTION AGENCY               *
*                                                               *
*****************************************************************

                    PRESS RETURN TO CONTINUE
```

Figure 14. Initial FLOWTHRU screen title, which appears at program start.

(Although the interactive mode can be somewhat more tedious to use, it does provide the user with the opportunity to run FLOWTHRU if an interprocess control file has not been created.)

3. Now enter a data output file name to be written or press <Enter> for the default name (Fluor_time.cnv) as requested. Be aware that previous output files can be overwritten if the same name is used for more than one. However, the input file previously entered cannot be overwritten if it is mistakenly reentered.

4. Enter a background file name to be written or press <Enter> for NULL, which means that no plot file is to be written (Figure 14). As with the output file name, duplicate usage of plot file names will result in the overwriting of previous plot files, but existing input file names will not be accepted. There is no default plot file name used (the default is no plot file). If a plot file name is given, then two plot files will be created: a time-concentration data file and a PostScript plot file. The latter will have an appropriate name assigned (e.g., *sampling station name*) and a .EPS extension added.

4.3. COMPUTER GRAPHICS

A high-quality color graphics algorithm, PGPLOT[11] (Pearson, 1997), which allows cascading graphics screens, direct printing, creation of screen files, and more using pull-down menus in the Windows environment, is included in FLOWTHRU. 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, and bitmapped plot files may be created "on the fly" using the pull-down menus.

4.3.1. Features of the Interactive Graphics Loop

Running FLOWTHRU will start a conventional Windows screen with a series of pull-down menus (Table 5). Each underlined character in Table 5 indicates that the <Alt> key plus the underlined character implements the respective menu item. For example, <Alt+F> will initiate 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 very often. Most of the more useful graphics functions have been built directly into FLOWTHRU so as to

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

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alleviate excess work on the part of the user. However, in some instances, the user may find particular functions of value.

The items shown in Table 5 work whether the program is currently at the text-only screen (Graphic 1), where the user responds to queries posed by FLOWTHRU, or whether the program is currently at the data-plot screen (PGPlot Graphics, #1). However, there is little point in accessing any of the pull-down items from the text-only screen, whereas in the data-plot screen the user may find some items of value. For example, the color data-plot screen can be printed as it appears, saved as it appears, resized to fit the whole screen, and so on.

A brief description of each pull-down item shown in Table 5 is provided in the next six subsections. Because the items are relatively self-explanatory, they are only described briefly.

4.3.1.1. *Interactive Data Point Deletion.* FLOWTHRU has also been programmed to allow the user to selectively remove specific data points. This is not a feature that should be used commonly, but there may be instances in which the user suspects the displayed data point in anomalous (e.g., as may occur due to a power surge). It is not a sophisticated routine, it does not always work as desired, and it should be used with considerable caution.

To selectively remove a specific data point, the user will place the cursor with cross-hairs over the data point to be removed. Due to the sensitivity of this routine, the user must be very precise in cursor placement so that the correct point is directly under the cursor (note that FLOWTHRU may still interpret cursor placement as a point other than that chosen by the user).

Pressing any appropriate keyboard key (e.g., an asterisk [*]) will mark the data point that FLOWTHRU plans to delete. The marked data point may or may not be the exact data point selected by the user. Because FLOWTHRU might mark an incorrect data point, the user is required to respond positively to a FLOWTHRU request to proceed with the data point deletion. To confirm deletion, the user must first press "Y", and <Enter> will delete the select data point and redraw the graph (note that case does not matter, Y = y and N = n). Pressing "N" and <Enter> will not delete the selected data point. To select another data point, the user must move the cursor back to the graphic window and press the Left Mouse Key to activate the graphic window. The actual process of data point deletion is as follows:

1. After the plot window appears, the user should enlarge the plot screen by *Left Clicking* on the "box" in the upper right-hand corner of the screen.

2. Next the user should place the cursor on the blue border at the top of the plot window, press and hold the left mouse button and drag the plot slightly to the right and down so as to

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display the text window, where the user will note some basic instructions.

3. At this point the user places the cursor and cross-hairs over a data point on the plot window to be deleted and presses any keyboard key *except* the slash (/). The data point to be deleted is now marked on the plot window and the data coordinates are shown on the text window with a request confirm deletion.

4. To confirm deletion or cancel deletion, the user must move the cursor over the text window and *Left Click* anywhere on the text window to make it active. The user may then enter a "Y" to confirm deletion or an "N" to cancel deletion followed by the "Enter" key to accept the command.

5. Entering Y and pressing Enter brings up a requestor asking for the Enter to be pressed again, which redraws the plot window with the deletion in effect.

6. Entering N and pressing Enter cancels the deletion process and restarts the cross-hair on the plot window.

7. To select additional points for deletion, the user must move the cursor back over the plot window and *Left Click* anywhere on the plot window to make it active.

8. This process may continue as long as the user wants to continue selecting data points for deletion.

9. At this point the original decimal time-concentration file and PostScript plot file (if one was to be created) have not been changed. To make the changes (deleted data points) take effect, the user must place the cursor anywhere over the plot window and press either the slash (/) or simultaneously press Ctrl-D or Ctrl-Z.

10. The user will see a message asking the user to press the Enter key. However, the user must first make the text window active by *Left Clicking* anywhere on the text window. Pressing Enter then makes all the changes effective and causes FLOWTHRU to proceed to end of the program, where the last basic commands are displayed.

It will be noted that the decimal time-concentration file and, if requested, a PostScript plot file will already have been created prior to the interactive routine having been implemented. Although many data points may have been selectively deleted, no final effect on any formal output files has

been performed at this stage. The user may kill the program at this stage by moving the cursor over the cross ($\times$) in the upper right corner of the screen and pressing the Left Mouse button.

To have FLOWTHRU formally accept all the deleted data points and create a final output file and/or PostScript plot reflecting these deletions, the user must enter either a slash (/) or simultaneously press `Ctrl-D` or `Ctrl-Z`. FLOWTHRU will then update all files reflecting all the deletions and proceed to the end of the program.

As a final note, it is not possible to delete the first data point, which always represents the time of tracer release ($t = 0$). To be correct, all tracer tests obviously always begin at the time of tracer release which must be taken as zero time.

4.4. FLOWTHRU SOURCE

The FORTRAN source for FLOWTHRU is included on the CD. It is a fairly large program and was split into pieces to allow for easier reading. It is not recommended that users attempt to follow the logic or modify the program. Questions regarding the program's functionality can be addressed to the author.

In addition, the graphics routine developed at the California Institute of Technology is included; however, it is not allowed for use in commercial products.

Table 5. Pull-down menu items available in FLOWTHRU.

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			Input	
	Paste			Clear Paste	
				Status Bar	
				1Graphic 1	
				2PGPlot Graphics, # 1	

File

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

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.*

Copy Ctrl+Ins *Copy selected items to the clipboard.*

Paste *Paste selected items to the screen.*

View

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

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

State

Pause Ctrl+S *Pause the graphic display.*

Resume Ctrl+Q *Resume graphic display.*

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

Windows

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* FLOWTHRU.

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

Contents *Listing of available help contents.*

Using Help *Description on the use of Help.*

About *Identifies the* FLOWTHRU *program.*

5. EXAMPLE RESULTS

The program FLOWTHRU is designed to produce decimal-time concentration data files and plots quickly and easily. Input by the user can be by the somewhat tedious method of interactively entering responses to questions posed by FLOWTHRU or by entering an interprocess-control file. (See Section 3.1. on page 18 for a detailed description of how FLOWTHRU uses an interprocess control file and Figure 9 on page 20 for an example process control file.) In the following examples, all production was accomplished using a process control file.

5.1. PROCESSING SIMPLE DATA FILES

A simple Turner Designs data file is a file, for the purposes of this section, that does not exhibit any interruptions in the file. A typical interruption in a Turner Designs data file would be a result of separate data blocks that have occurred as a result of a scheduled fluorescence data logging. Two simple Turner Designs data files are included here.

5.1.1. Turner Designs Data File Tracq01.prn

The data file Tracq01.prn[12], was produced from a column test with the fluorometer logging data every second. The entire column experiment lasted a little more than 18 minutes. Figure 15 is a plot of the time-concentration data file using decimal minutes. From Figure 15 a number of things are apparent. First, all the data lie significantly above zero concentration. Data recording actually coincided with tracer injection, so no background concentrations were produced. To evaluate this data set using a program such as QTRACER2, some "representative" value for background concentration should be developed using the first seven minutes.

The second apparent item is that considerable noise occurs in the data when the logger is set to record as frequently as every second. Although the data, as is, can be processed using any number of different modeling packages, it might be desirable to have a smoothing algorithm (e.g., Moving Average Filter, Convolution, etc.) applied to the data to remove the excess noise (see Section 5.1.3.).

The third apparent item is that there are so much data recorded in Figure 15 it is very difficult to identify any specific features in the plot. This problem can be overcome by having FLOWTHRU process a percentage of the data, which will also cause a decrease in the amount of noise in the

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[12]Data file, Tracq01.prn was developed by Anne Motelay-Massei and provided by Nicolas Massei of the Département of Géologie, Université de Roun.

data. However, processing just a percentage of the data may cause unwanted aliasing, which must be considered by the user. Figure 16 is a plot of ~20% of the data.

A close visual inspection of Figures 15 and 16 suggests that there is no significant difference between the two plots. However, a data-analysis or modeling package (e.g., QTRACER2 or CXTFIT2) is needed to verify that any differences are minor (as was done in this report in Sections 5.1.3.2. on page 53 and 5.1.3.3. on page 59). Figure 16 could be displayed with even less data to allow additional clarity.

For example, Figure 7 on page 16 shows just 0.7% of the data provided in Figure 1 on page 3[13]. Processing just 0.7% of the data was determined by FLOWTHRU because an exact match to every decimal day was requested.

5.1.2. Turner Designs Data File Tracq04.prn

The data file Tracq04.prn[14] was produced from a column test with the fluorometer logging data every second. The entire column experiment lasted a little less than 9 minutes. Figure 17 is a plot of the time-concentration data file using decimal minutes. Like Figure 15, Figure 17 also shows that all the data lie significantly above zero concentration. Again, data recording coincided with tracer injection, so no background concentrations were produced. Breakthrough curve evaluation requires that some "representative" value for background concentration be developed from the first two minutes.

In addition, considerable noise occurs in the data shown in Figure 17 when the logger is set to record as frequently as every second, just as occurred in Figure 15. However, Figure 17 also exhibits extreme noise at the very start of the BTC, which could be "real" or may be leftover tracer from a previous tracer test that was sorbed onto particles making up the porous media in the column. In order to better study Figure 17, a reduced data set can be plotted, as was done with the Tracq01.prn data in Figure 16. Figure 18 is a plot of just 10% of the Tracq04.prn data with data averaging. The error bars included in Figure 18 provide an indication of the effect of data averaging, which is extreme at the beginning of the file and not so significant as the "real" data are processed. It is up to the user to determine whether data averaging is appropriate.

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[13]The full data file Fluor_Time.prn is on the enclosed CD and is a default file used by FLOWTHRU for testing.

[14]Data file Tracq04.prn was developed by Anne Motelay-Massei and provided by Nicolas Massei of the Département of Géologie, Université de Roun.
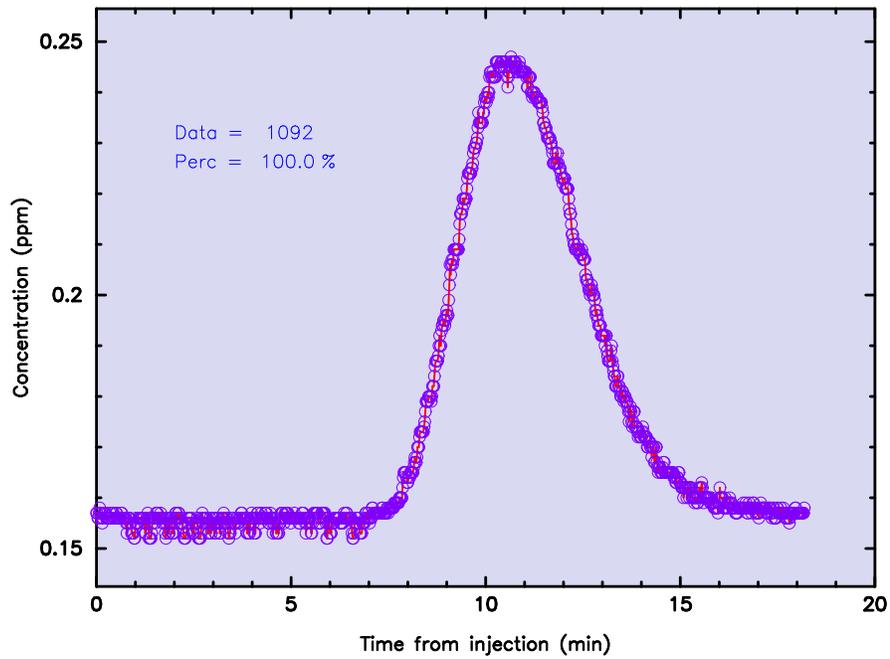
Figure 15. Decimal time-concentration data file for the Tracq01.prn data file developed from a short-term column study (100% of the data shown).
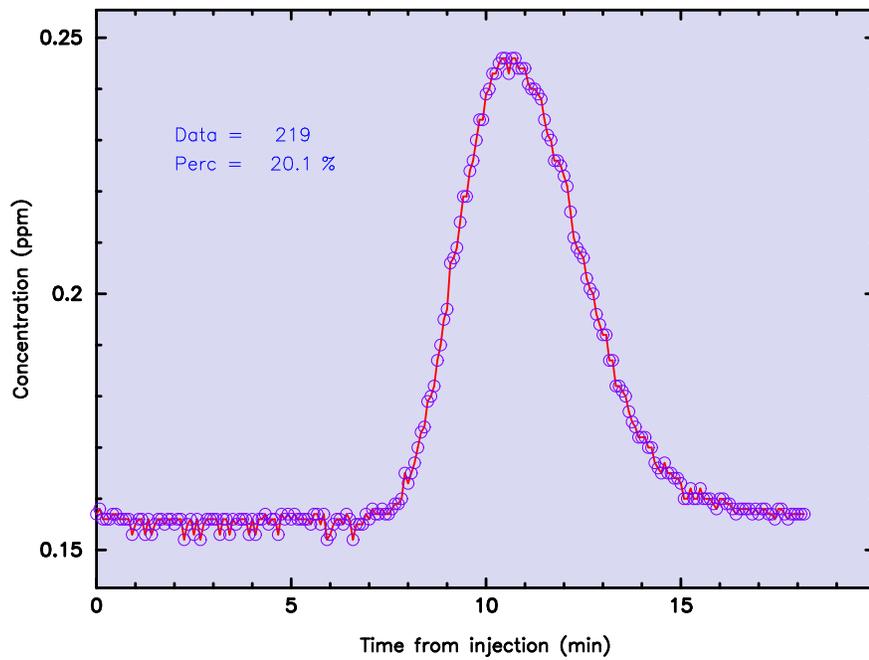
Figure 16. Decimal time-concentration data file for the Tracq01.prn data file developed from a short-term column study (20.1% of the data shown).
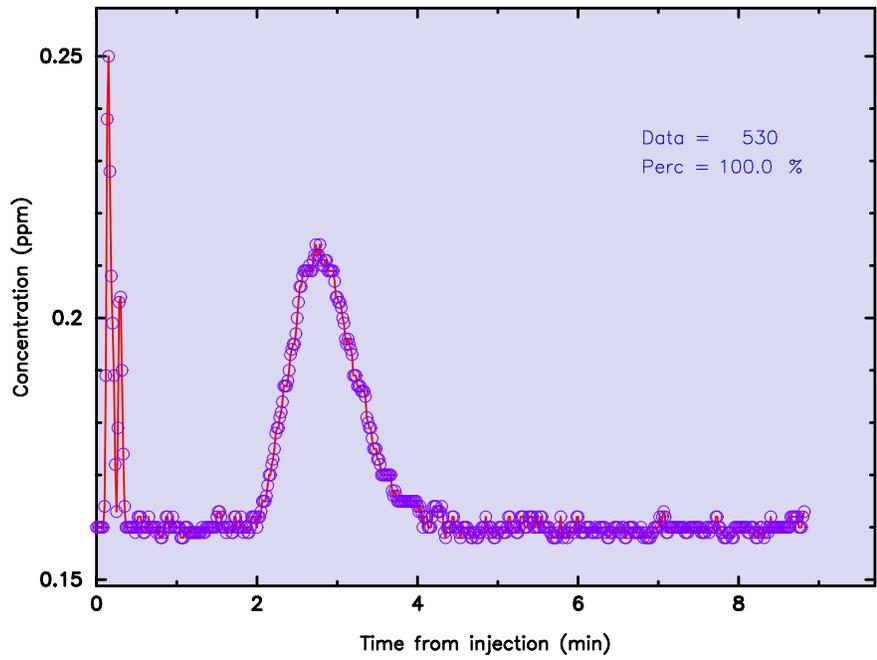
Figure 17. Decimal time-concentration data file for the Tracq04.prn data file developed from a short-term column study (100% of the data shown).
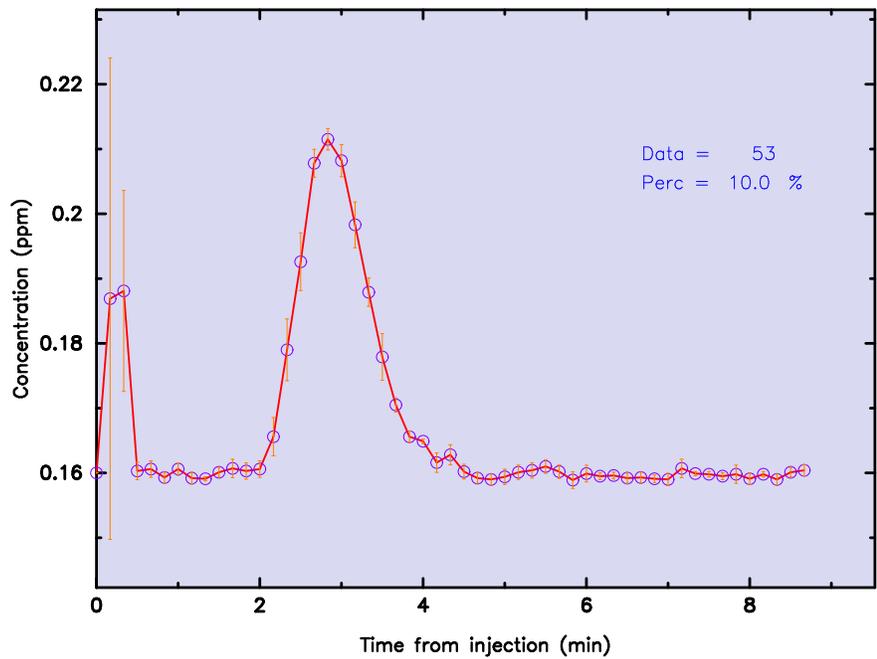
Figure 18. Decimal time-concentration data file for the Tracq04.prn data file developed from a short-term column study (10% of the data shown). Note error bars indicating the effect of averaging.

5.1.3. Moving Average Filter Effect on a Data File

In Section 5.1.1., it was suggested that use of a moving average filter (or similar operation) as a means for smoothing data logged on an extremely frequent basis (e.g., every second) might be desirable in rare instances. Tracer data smoothing is generally not recommended, but a moving average filter (Brandt, 1999, pp. 427–440) has been included in the FLOWTHRU package for those instances where data smoothing may be desirable. Both the Tracq01.prn and Tracq04.prn data sets exhibit a significant amount of noise as a result of the frequency of data recording (every second), so a data-smoothing operation might be desirable for these two data sets. The moving average filter routine included in FLOWTHRU has been applied to the Tracq01.prn and Tracq04.prn data sets so that the smoothing effect may be observed.

Figure 19 is a plot of smoothed Tracq01.prn decimal time-concentration data. Comparing Figure 19 with Figure 15 on page 49 suggests that in this particular instance a moving average filter might be desirable.

Figure 20 is a plot of smoothed Tracq04.prn decimal time-concentration data. The 95% confidence limits for the smoothed decimal time-concentration data file for the Tracq04.prn data are also shown in Figure 20 (orange lines in Figure 20). The confidence limits stand out at the early-time data but cannot be observed for the rest of the data. This suggests that although much of the smoothed data vary minimally from the real data, the early-time data developed substantial errors when smoothed. Figure 19 also has the 95% confidence limits plotted for the smoothed data, but the errors are so minimal the confidence limits cannot be observed.

Comparing Figure 20 with Figure 17 suggests that in this particular instance a moving average filter might not be quite as desirable because of the early-time "noise" in the Tracq04.prn data file. The effect of this early-time noise is reflected in the 95% confidence level (orange lines in Figure 20). Both Figures 17 and 20 indicate that the early-time data in this file represent a special problem that needs to be considered.

Peak concentration equals 0.212–0.214 ppm (after subtracting $\overline{C}_b = 0.160$ ppm) for the data shown in Figure 17 (see Sample Numbers 165–168 in Appendix I on page 81) and 0.212 ppm for the smoothed data shown in Figure 20 (see Sample Numbers 167–176 in Appendix I on page 81). This net difference of 0.000–0.002 ppm, although carried through the smoothed data, may not represent a substantial error when a quantitative analysis of the BTC is performed. The same may not be said for the Tracq01.prn data set, where peak measured concentration equals 0.246 ppm for the data shown in Figure 15 and 0.246 ppm for the smoothed data shown in Figure 19 for a net difference of 0.000 ppm (after subtracting $\overline{C}_b = 0.156$ ppm).
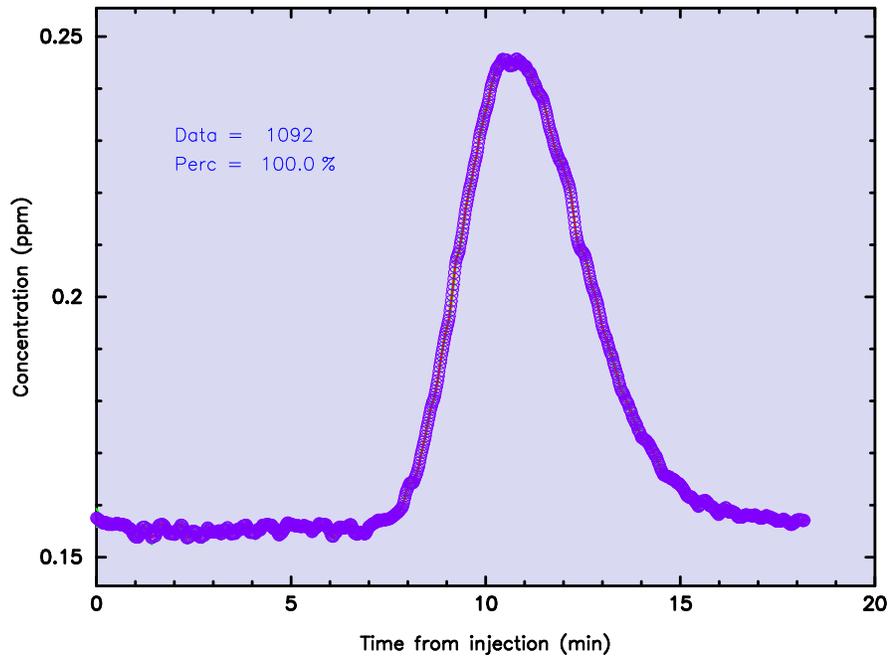
Figure 19. Smoothed decimal time-concentration data file for the Tracq01.prn data file developed from a short-term column study (100% of the data shown).
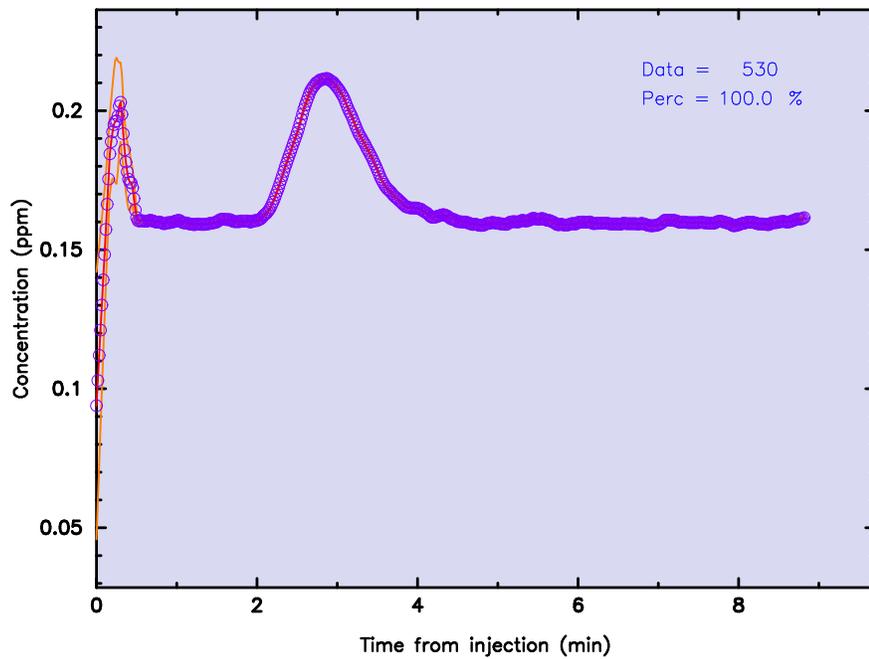
Figure 20. Smoothed decimal time-concentration data file for the Tracq04.prn data file developed from a short-term column study (100% of the data shown). Note confidence limits shown in orange.

In addition, Figure 15 shows that the peak time of arrival occurred at 10.53 min after injection, whereas Figure 19 shows that peak arrival occurred at 10.60 min (a net difference of 0.07 min). Figure 17 shows that the peak time of arrival occurred at 2.733–2.783 min, whereas Figure 20 shows that peak arrival occurred at 2.867 min (a net difference of $0.134 - 0.084$ min). These time shifts in the smoothed data suggest the possibility that some time-of-travel error (significant or otherwise) may be evident. These differences in travel times, although small, may be critically important when modeling solute transport times. Such differences in travel times can have major consequences and must be regarded very carefully. In these two instances, both smoothed data files indicate slower transport times for peak concentrations than that which was measured, but modeling efforts need to be conducted to determine the significance of the slower transport rates.

5.1.3.1. *Absolute and Relative Smoothing Errors.* The differences observed between the measured data and the smoothed data for the Tracq01.prn and the Tracq04.prn data sets are better illustrated in Figures 21 and 22, respectively. The absolute errors between the measured concentrations and the smoothed concentrations acquired from the moving average are calculated by

$$\text{absolute error} = \text{true value} - \text{approximate value} \tag{4}$$

and the relative errors between the measured concentrations and the smoothed concentrations acquired from the moving average are calculated by

$$\text{relative error} = \frac{\text{absolute error}}{\text{true value}} \tag{5}$$

The absolute and relative errors between the measured BTC and the smoothed BTC for the Tracq01.prn data set are illustrated in Figures 23 and 24, respectively. The absolute and relative errors shown in Figures 23 and 24 appear amplified as a result of the scale chosen.

The absolute and relative errors between the measured BTC and the smoothed BTC for the Tracq04.prn data set are shown in Appendix I on page 81.Figures 25 and 26 are plots of the absolute and relative errors, respectively, between the measured BTC and the smoothed BTC for the Tracq04.prn data set.

5.1.3.2. FLOWTHRU *Analysis of the Measured and Modified Data Sets.* Before the averaged or smoothed data sets can be accepted, a careful evaluation of the averaging and smoothing effects should be conducted. To evaluate the averaging and smoothing effects here, the QTRACER2 program (Field, 2002) was used. First, the measured data were evaluated using QTRACER2 and
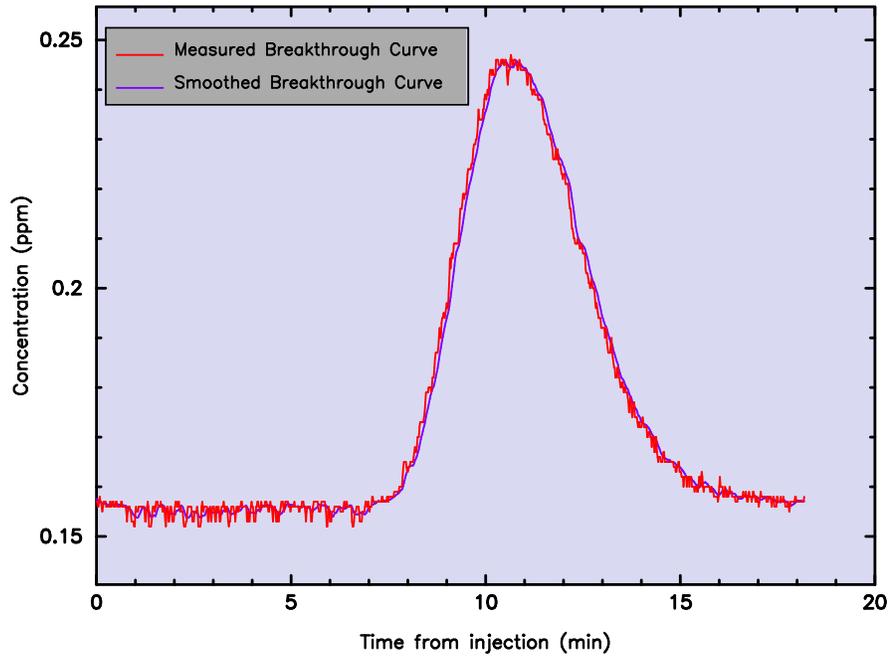
Figure 21. Comparison of measured and smoothed concentrations Tracq01.prn data file.
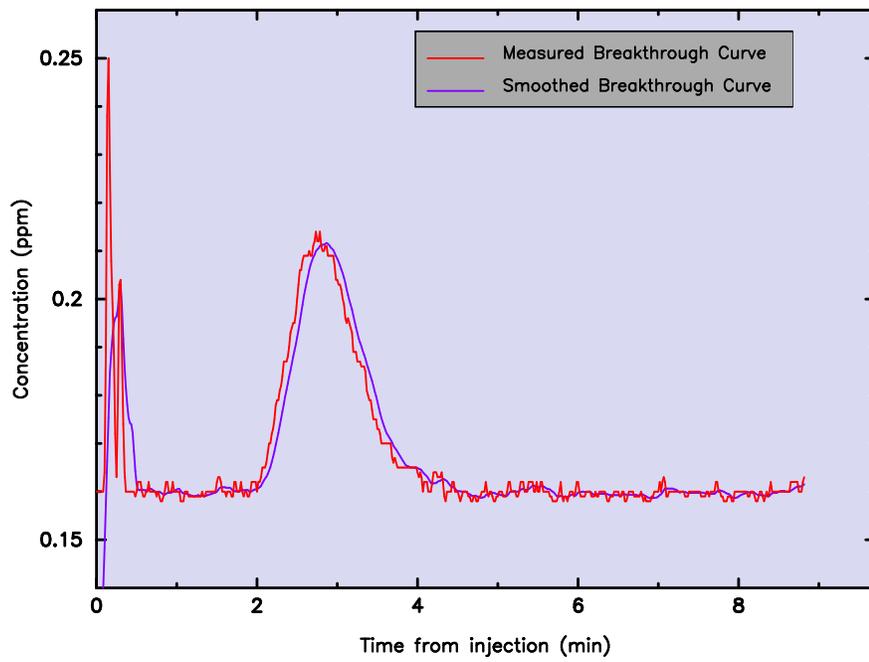
Figure 22. Comparison of measured and smoothed concentrations Tracq04.prn data file.
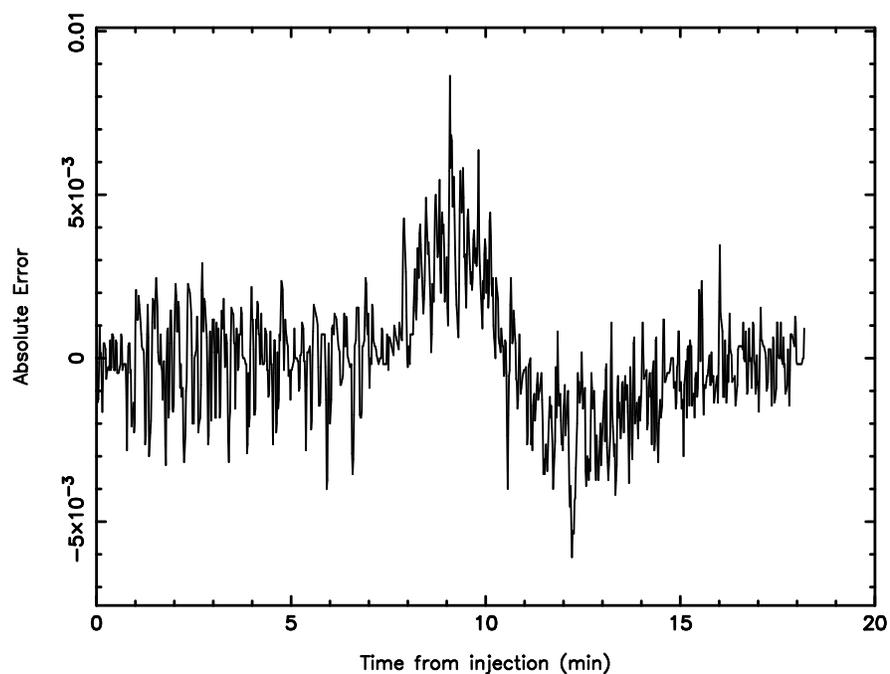
Figure 23. Plot of absolute errors between measured and smoothed concentrations for the Tracq01.prn data file.
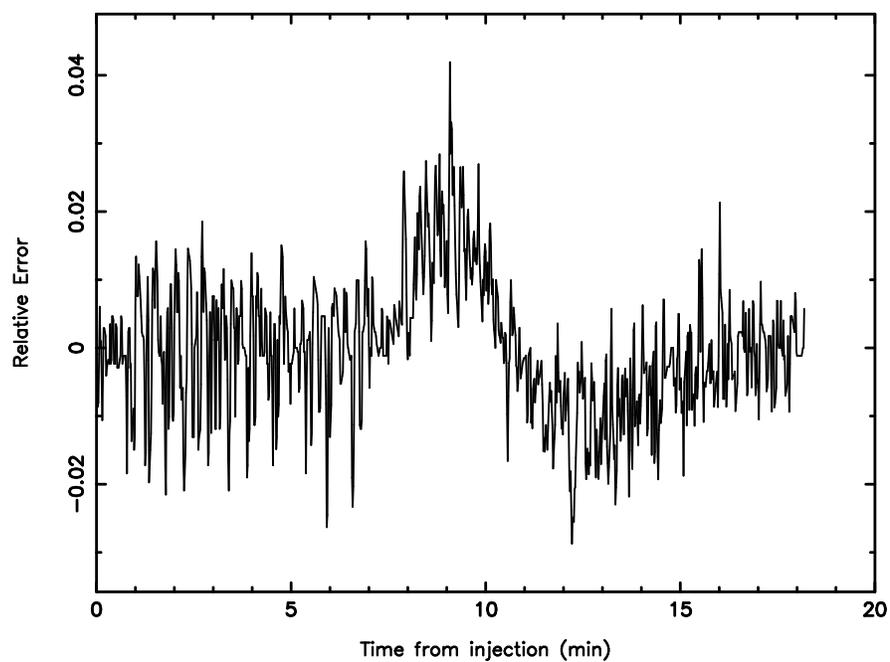
Figure 24. Plot of relative errors between measured and smoothed concentrations for the Tracq01.prn data file.

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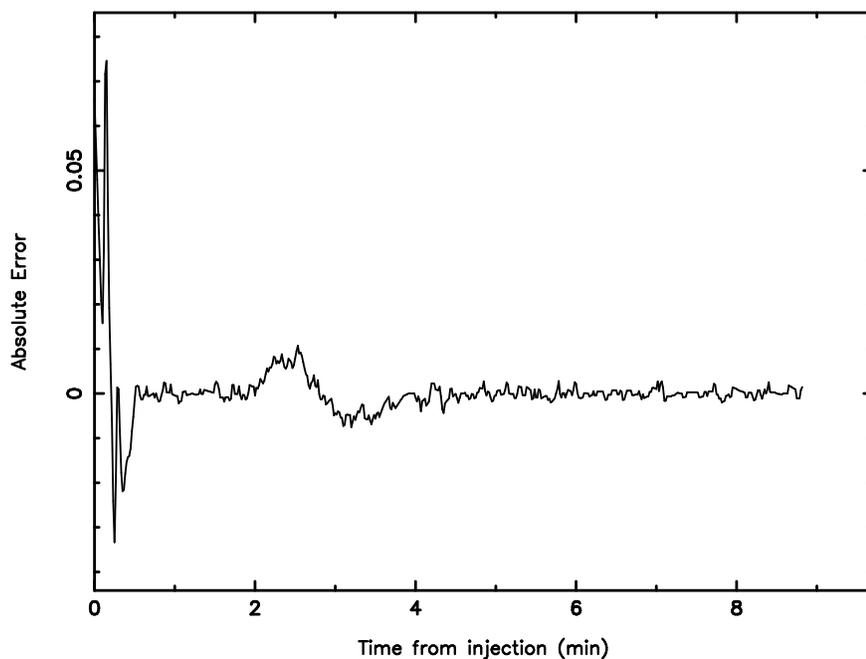
Figure 25. Plot of absolute errors between measured and smoothed concentrations for the Tracq04.prn data file.
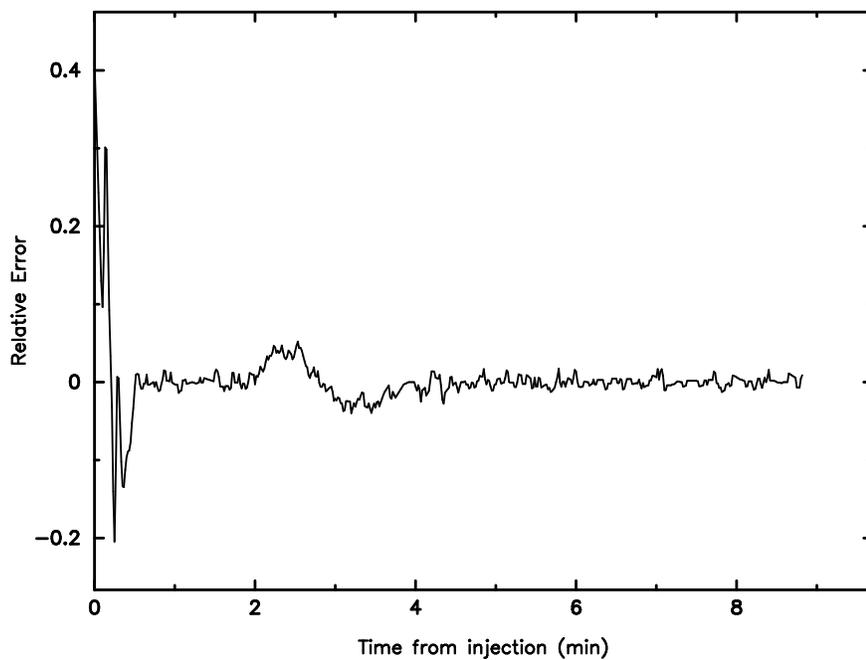
Figure 26. Plot of relative errors between measured and smoothed concentrations for the Tracq04.prn data file.

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Table 6. Evaluation of measured and modified concentration parameters for Tracq01.prn.

Data Set	Mass Recovered (μg)	Percent Recovered (dimen.)	Time to Peak (seconds)	Peak Concentration (ppm)
Measured	35.099	99.997	639.000	0.091
Averaged[a]	35.157	100.160	640.000	0.091
Smoothed	35.002	99.722	626.000	0.090

[a] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.006$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.156$ ppm (subtracted from data file).

Table 7. Evaluation of measured and modified transport parameters for Tracq01.prn.

Data Set	First Arrival[a] (seconds)	Mean Travel Time (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet No. (dimen.)
Measured	0.0000	667.320	0.00180	2.10×10^{-5}	102.68
Averaged[b]	0.0000	667.440	0.00180	1.51×10^{-5}	143.10
Smoothed	0.0000	673.260	0.00178	2.12×10^{-5}	100.91

[a] Residual tracer in the system incorrectly causes an apparent first arrival equal to injection time.
[b] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.006$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.156$ ppm (subtracted from data file).

then the averaged and smoothed data were evaluated. The evaluation results for the Tracq01.prn data set are shown in Tables 6 and 7 and the evaluation results for the Tracq04.prn data set are shown in Table 8 and 9.

Table 6 shows that the results of both the averaged and the smoothed data sets reasonably match the measured results even though a slightly greatermass of dye was recovered for the averaged concentrations. Table 7 also shows acceptable matches between the averaged and smoothed data sets with the measured data set. Only the mean travel time and axial dispersion values for the smoothed data set deviate to any significant degree from the measured data set.

Tables 8 and 9 are more interesting than Tables 6 and 7 because the smoothed data sets show what might be considered better parameter estimates for peak time of arrival t_p, axial dispersion

Table 8. Evaluation of measured and modified concentration parameters for Tracq04.prn.

Data Set	Mass Recovered (μg)	Percent Recovered (dimen.)	Time to Peak (seconds)	Peak Concentration (ppm)
Measured	25.343	100.010	9.002	0.090
Averaged[a]	25.284	99.779	10.002	0.079
Smoothed	24.913	98.313	172.000	0.052

[a] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.024$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.160$ ppm (subtracted from data file).

Table 9. Evaluation of measured and modified transport parameters for Tracq04.prn.

Data Set	First Arrival (seconds)	Mean Travel Time (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet No. (dimen.)
Measured	6.0017	152.808	0.00785	1.01×10^{-3}	9.35
Averaged[a]	6.0017	152.664	0.00786	9.77×10^{-4}	9.65
Smoothed	8.0017	156.552	0.00767	6.12×10^{-5}	150.35

[a] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.024$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.160$ ppm (subtracted from data file).

D_x, and the Péclet number P_e than did the measured or averaged data set. All three forms of the Tracq04 data sets resulted in approximately the same mass recoveries, first arrival times, mean time of travel, and mean velocity, but the similarities end there. The measured time to peak concentration ($t_p = 9.000$ s) and averaged time to peak concentration ($t_p = 10.002$ s) are clearly in error, whereas the smoothed time to peak concentration ($t_p = 172$ s $= 2.867$ min) is much more reasonable (see Figure 17 on page 50). The incorrect estimate for t_p for the measured data by QTRACER2 is a direct consequence of the extreme noise in the early-time data in Tracq04.prn and should be apparent when examining a plot of the data (Figure 17 on page 50). This early-time noise in the data could be manually corrected.

Additionally, the parameter estimates for the Tracq01 data sets may be taken as more reliable than the Tracq04 data sets for the flow system because the Tracq01 data sets do not have such

extreme early-time noise as the Tracq04 data sets. If this assumption is acceptable, then it follows that the estimates for axial dispersion ($D_x = 6.12 \times 10^{-5}$ m^2 s^{-1}) and Péclet number ($P_e = 150.35$) are more reasonable than are the estimates derived from the Tracq04 measured and averaged data sets.

5.1.3.3. CXTFIT2 *Analysis of the Measured and Modified Data Sets.* To further investigate the impact of smoothing data automatically logged by a Turner Designs Model 10-AU-005, CXTFIT2 (Toride et al., 1995) was run in the inverse mode for both the equilibrium and nonequilibrium models. The intent was to calibrate the FLOWTHRU-estimated parameters to theoretical models to see how well the modified data results matched measured data results.

Figures 27, 28, and 29 are plots of the equilibrium model fits to the measured, averaged, and smoothed Tracq01 data sets, respectively. Figures 30, 31, and 32 are plots of the nonequilibrium model fits to the measured, averaged, and smoothed Tracq01 data sets, respectively. All six model fits appear quite good visually.

Figures 33, 34, and 35 are plots of the equilibrium model fits to the measured, averaged, and smoothed Tracq04 data sets, respectively. Figures 36, 37, and 38 are plots of the nonequilibrium model fits to the measured, averaged, and smoothed Tracq04 data sets, respectively. Unlike the Tracq01.prn data sets (Figures 27–32), only Figures 35 and 38 appear good visually.

Parameter estimates for the equilibrium model fits for the Tracq01.prn and Tracq04.prn data sets are shown in Tables 10 and 11, respectively. The data shown in Table 10 show relatively little difference between the measured, averaged, and smoothed methods. However, the smoothed data shown Table 11 is much different than the measured and averaged data, which is a direct result of the improved model fitting that occurs with the smoothed data.

Parameter estimates for the nonequilibrium model fits for the Tracq01.prn and Tracq04.prn data sets are shown in Tables 12 and 13, respectively. Again, the smoothed data shown in Table 13 are very different from the measured and averaged data and represent an improvement.

5.2. PROCESSING MODERATELY COMPLEX DATA FILES

As described in Section 1.1.1. on page 2 the process of downloading a file to a computer from a Model 10-AU-005 by use of the program IDL_1B1 may result in a slight time break in the data file because of the necessity of shutting down the logger during file downloading. This slight time break must be properly identified and a correction included in the converted data file.
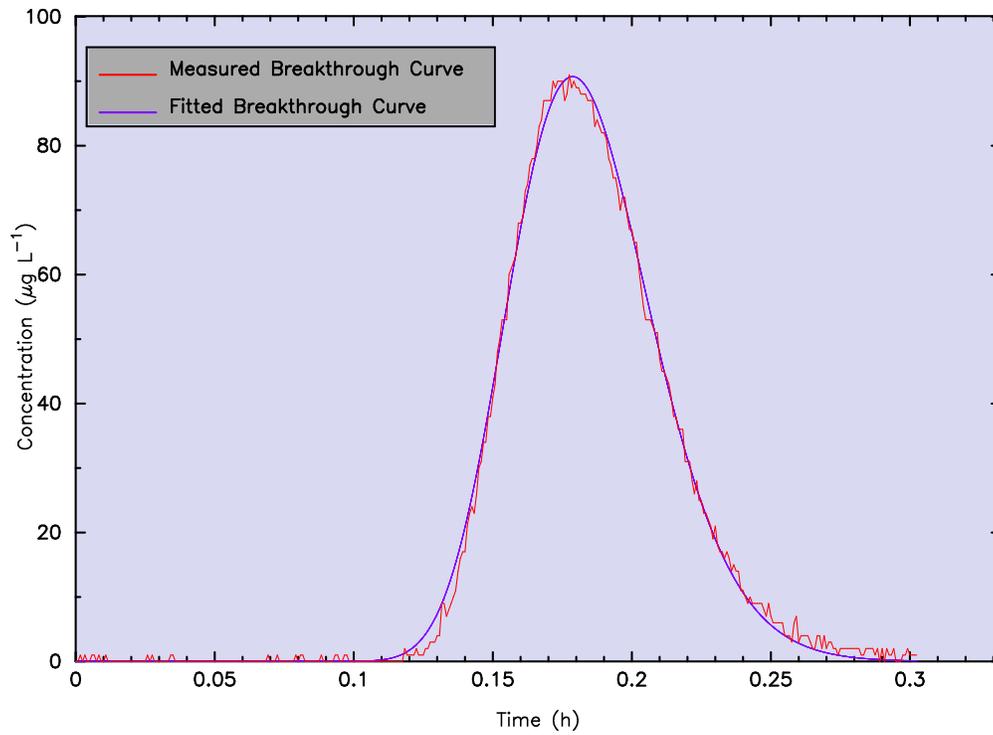
Figure 27. Plot of the equilibrium model fit to the measured Tracq01.prn data.
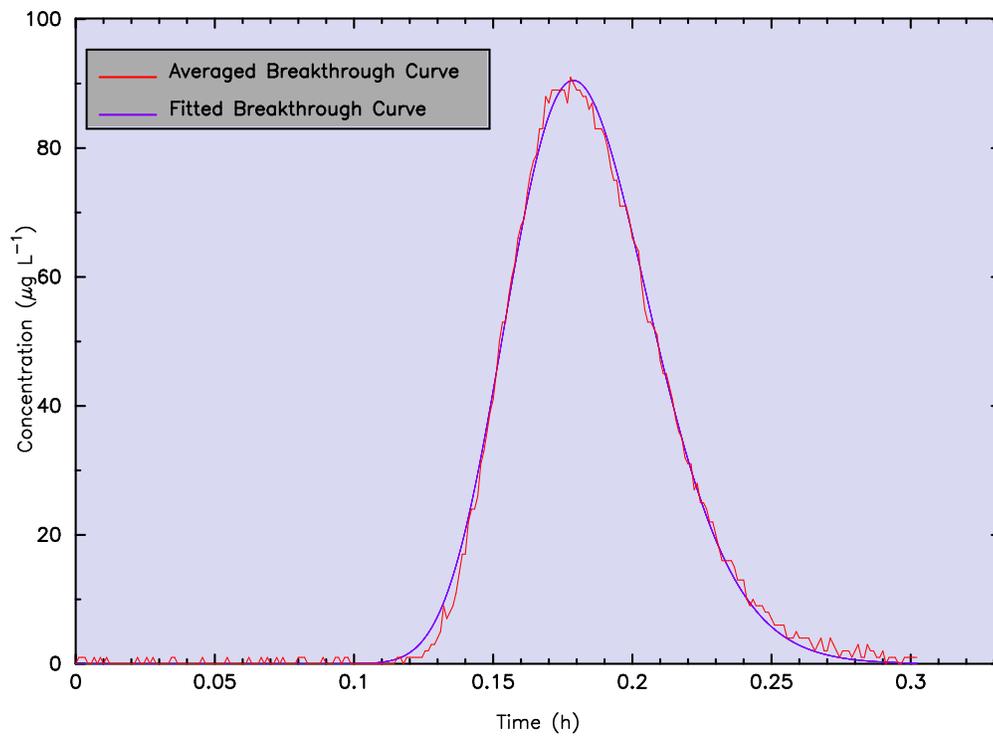
Figure 28. Plot of the equilibrium model fit to the averaged Tracq01.prn data.
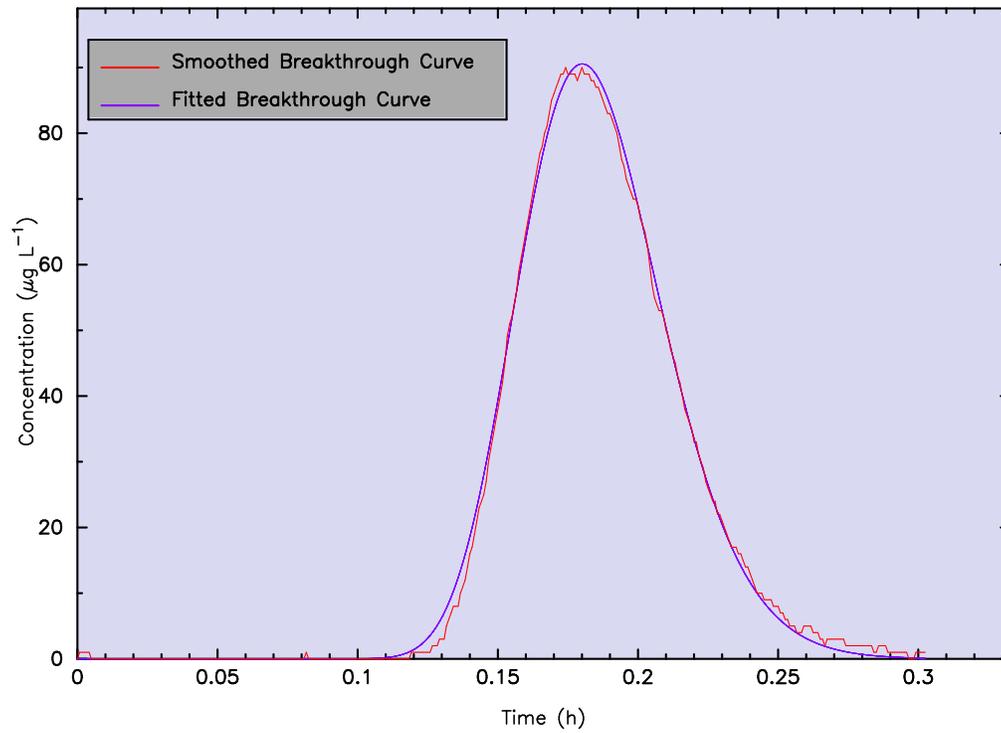
Figure 29. Plot of the equilibrium model fit to the smoothed Tracq01.prn data.
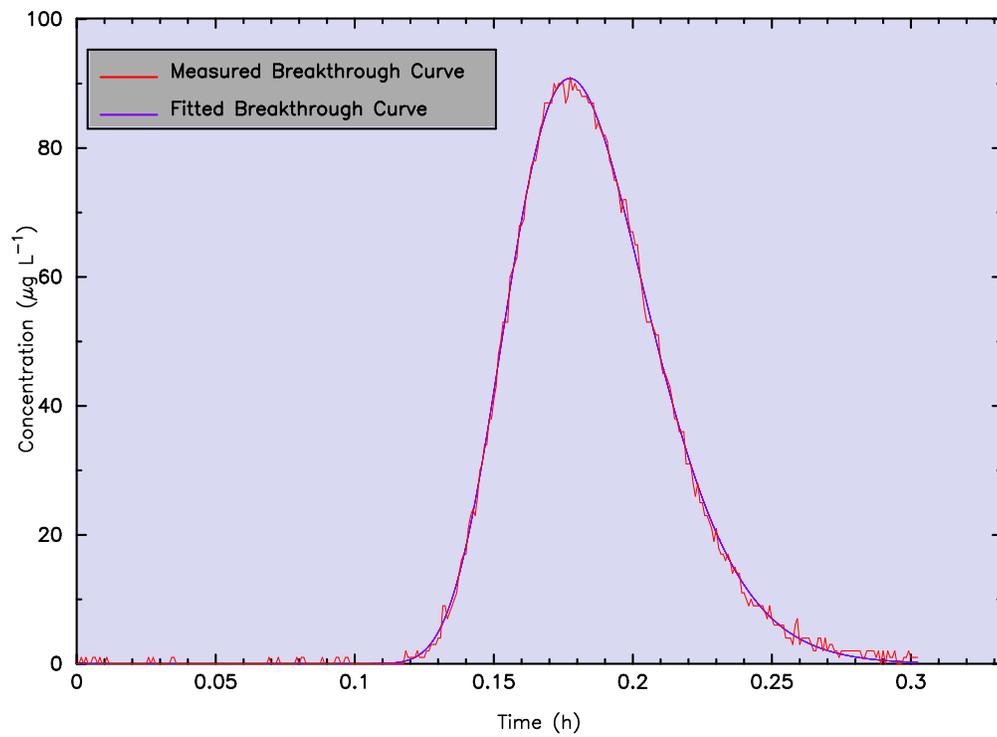
Figure 30. Plot of the nonequilibrium model fit to the measured Tracq01.prn data.
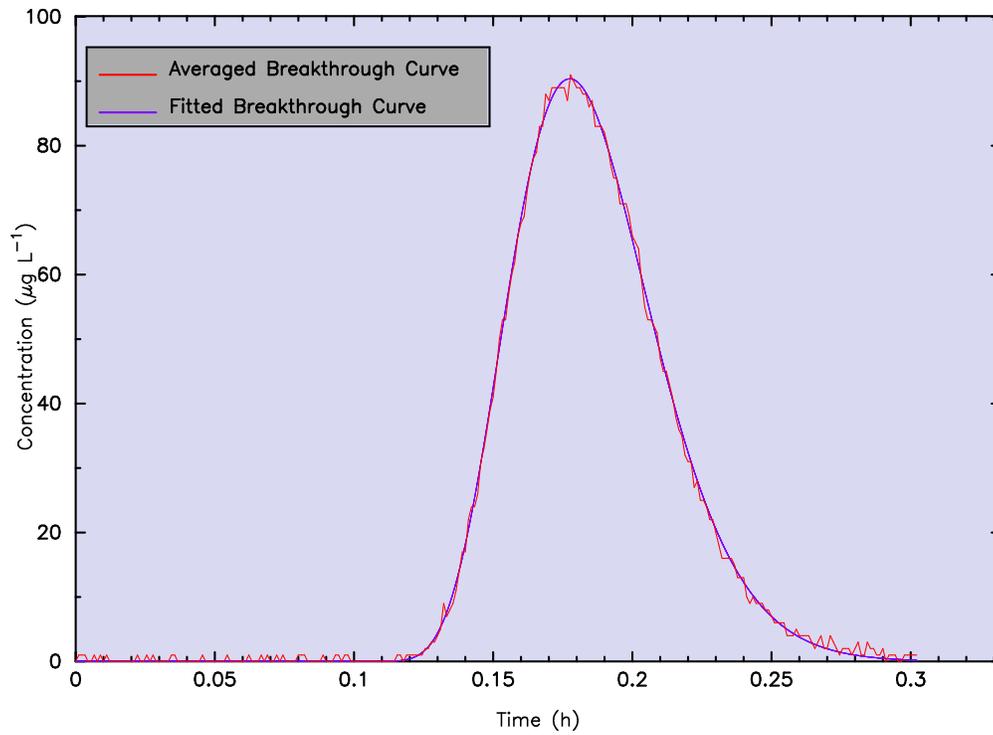
Figure 31. Plot of the nonequilibrium model fit to the averaged Tracq01.prn data.
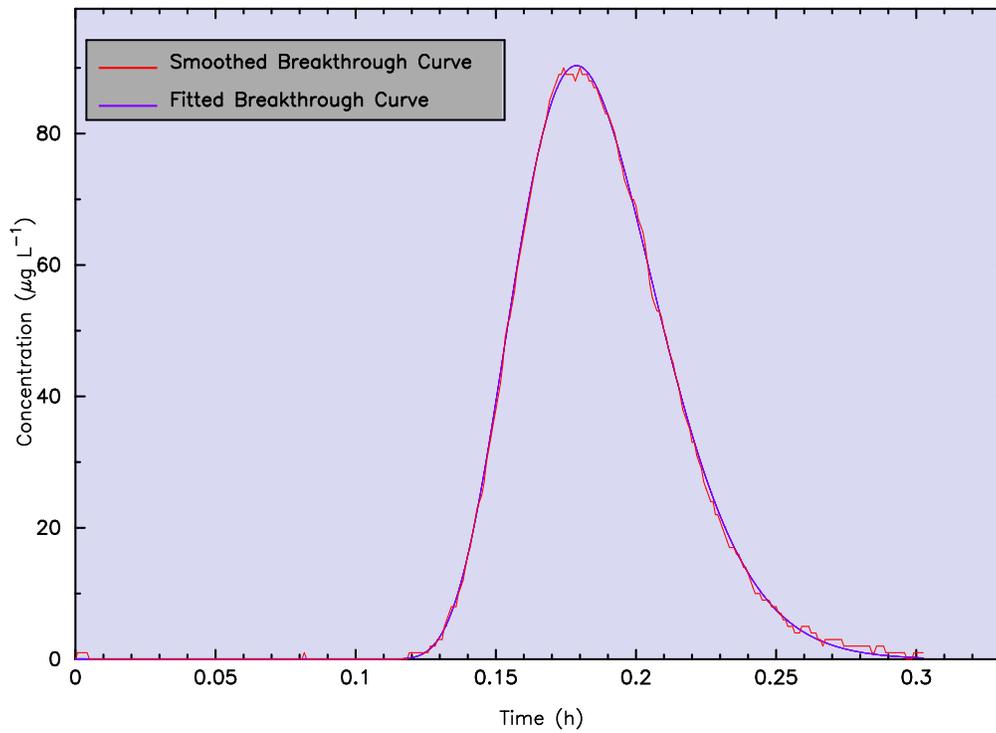
Figure 32. Plot of the nonequilibrium model fit to the smoothed Tracq01.prn data.
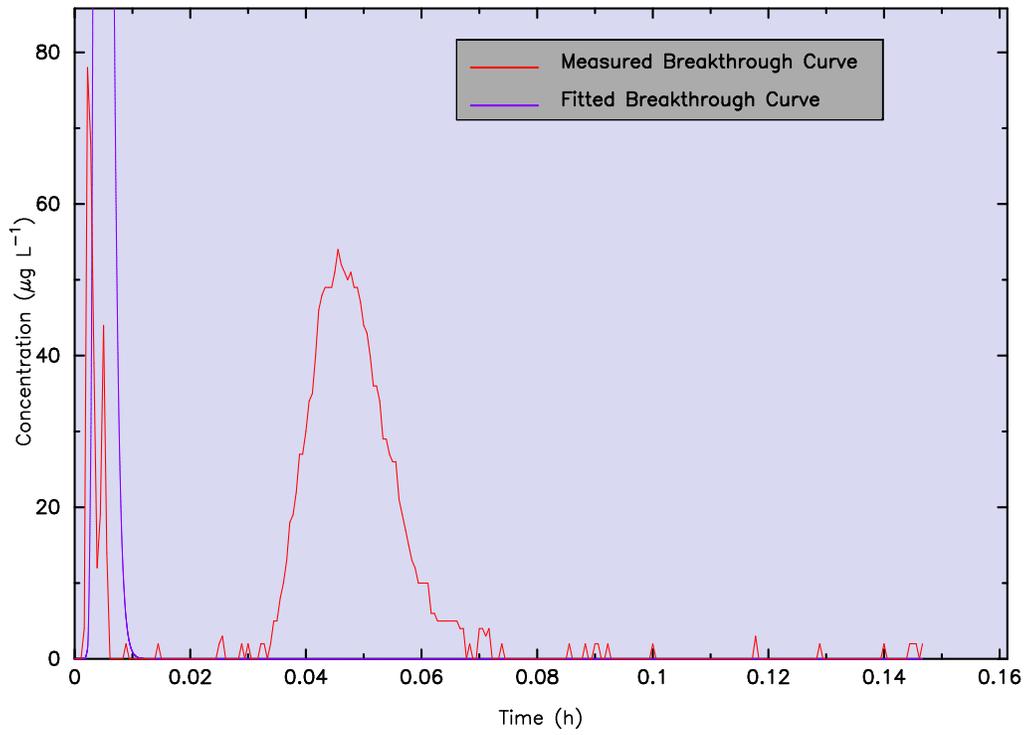
Figure 33. Plot of the equilibrium model fit to the measured Tracq04.prn data.
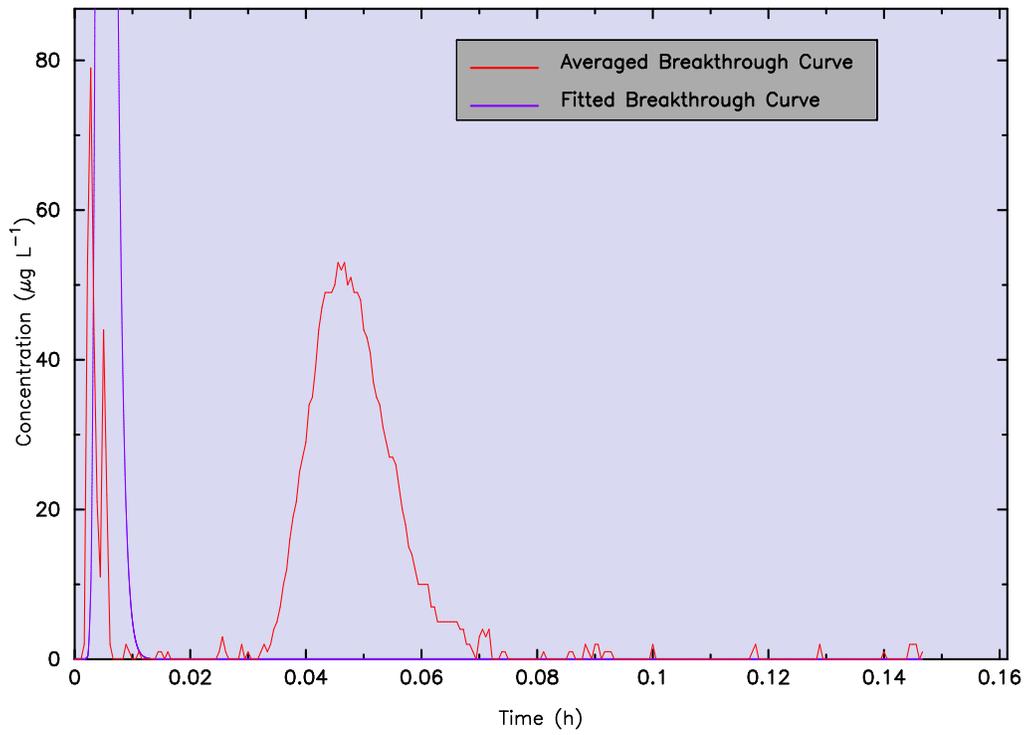
Figure 34. Plot of the equilibrium model fit to the averaged Tracq04.prn data.
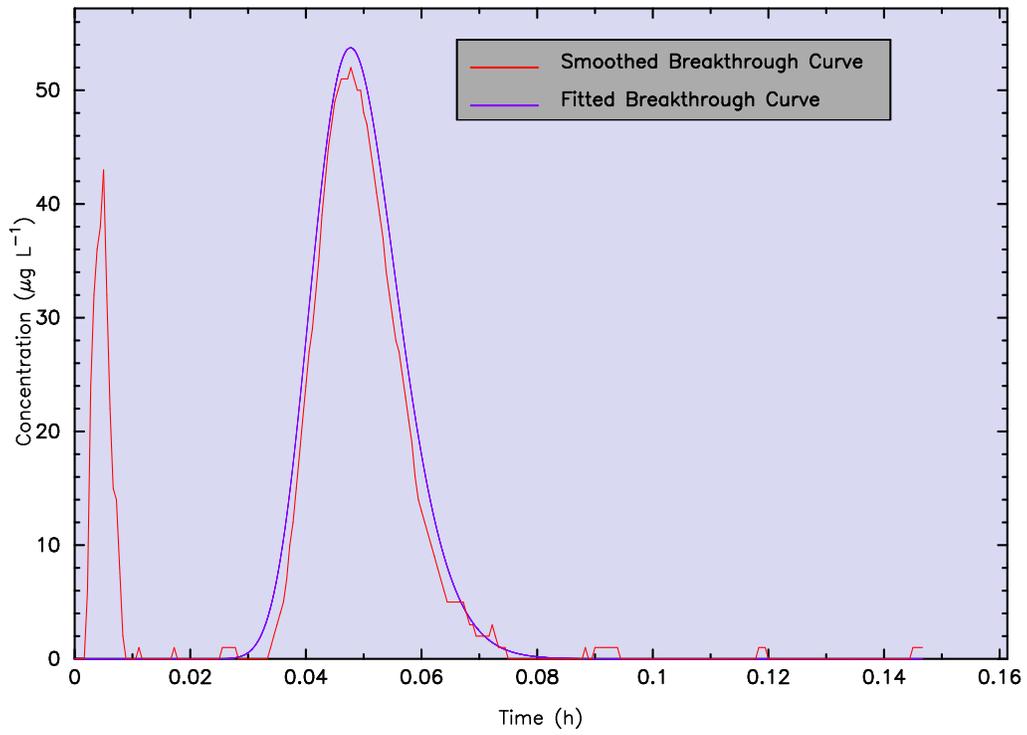
Figure 35. Plot of the equilibrium model fit to the smoothed Tracq04.prn data.
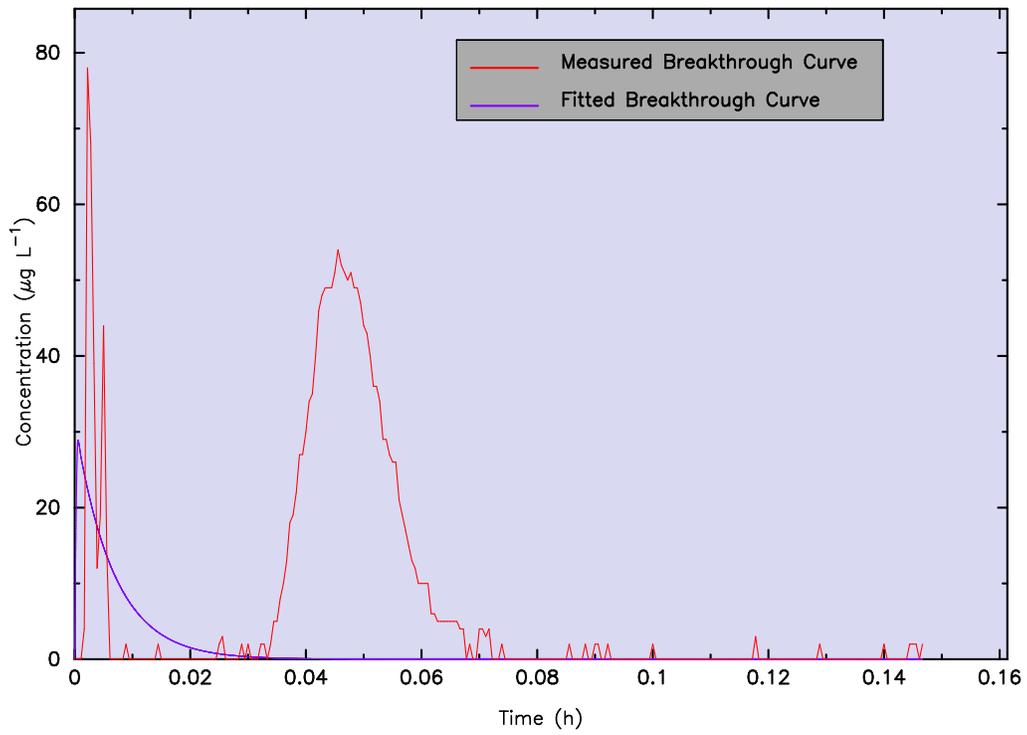
Figure 36. Plot of the nonequilibrium model fit to the measured Tracq04.prn data.
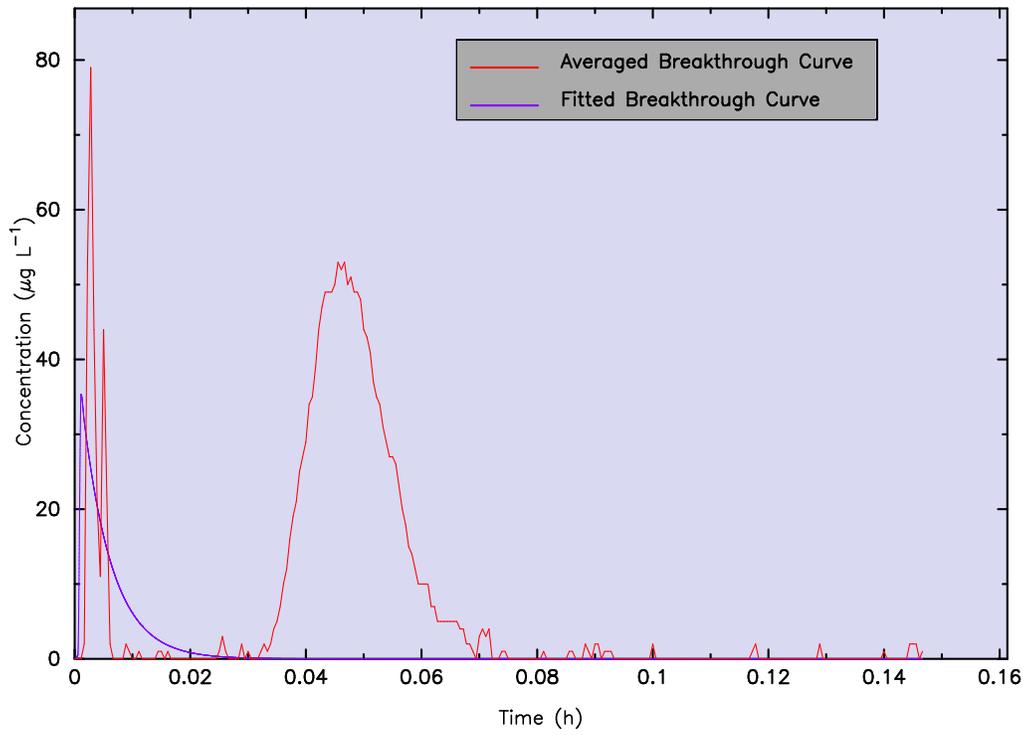
Figure 37. Plot of the nonequilibrium model fit to the averaged Tracq04.prn data.
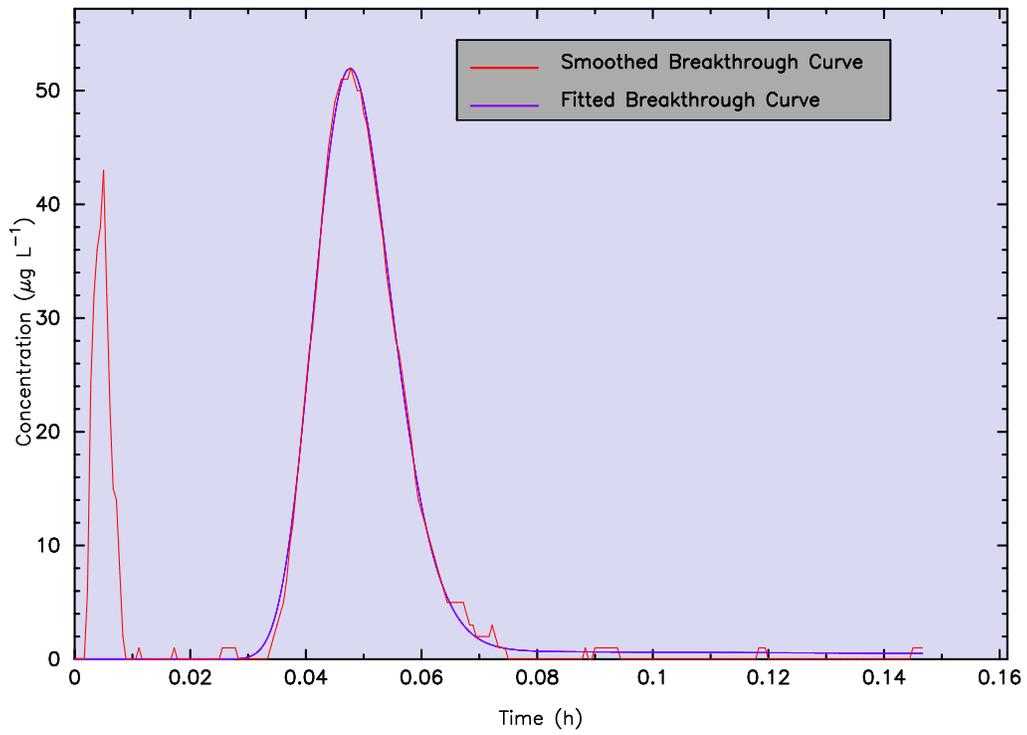
Figure 38. Plot of the nonequilibrium model fit to the smoothed Tracq04.prn data.

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Table 10. Evaluation of equilibrium model estimated transport parameters for Tracq01.prn.

Data Set	Mean Travel Time (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet No. (dimen.)	R^2
Measured	662.983	0.00181	2.22×10^{-5}	97.84	0.9977
Averaged[a]	662.983	0.00181	2.22×10^{-5}	97.84	0.9977
Smoothed	666.667	0.00180	2.17×10^{-5}	99.54	0.9981

[a] FLOWTHRU-determined percentage of data to process (= 50%).
   Transport distance $L = 1.20$ m.
   Discharge flow $Q = 0.006$ m^3 h^{-1}.
   Background concentration $\overline{C}_b = 0.156$ ppm (subtracted from data file).

Table 11. Evaluation of equilibrium model estimated transport parameters for Tracq04.prn.

Data Set	Mean Travel Time (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet No. (dimen.)	R^2
Measured	18.007	0.06664	2.02×10^{-5}	3.96×10^3	******
Averaged[a]	20.000	0.06000	1.95×10^{-3}	3.69×10^1	******
Smoothed	178.306	0.00673	9.71×10^{-5}	8.32×10^1	0.8247

[a] FLOWTHRU-determined percentage of data to process (= 50%).
   Transport distance $L = 1.20$ m.
   Discharge flow $Q = 0.024$ m^3 h^{-1}.
   Background concentration $\overline{C}_b = 0.160$ ppm (subtracted from data file).

Table 12. Evaluation of nonequilibrium model estimated transport parameters for Tracq01.prn.

Data Set	Mean Time of Travel (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet Number (dimen.)	Degree of Nonequilibrium (dimen.)	Mass Transfer Coefficient (h^{-1})	R^2
Measured	666.667	0.00180	9.62×10^{-6}	224.53	0.8303	4.740	0.9989
Averaged[a]	666.667	0.00180	3.67×10^{-6}	588.56	0.7118	9.564	0.9990
Smoothed	674.157	0.00178	3.01×10^{-6}	709.64	0.7027	10.000	0.9995

[a] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.006$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.156$ ppm (subtracted from data file).

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Table 13. Evaluation of nonequilibrium model estimated transport parameters for Tracq04.prn.

Data Set	Mean Time of Travel (seconds)	Mean Velocity (m s^{-1})	Axial Dispersion (m^2 s^{-1})	Péclet Number (dimen.)	Degree of Nonequilibrium (dimen.)	Mass Transfer Coefficient (h^{-1})	R^2
Measured	5.072	0.2366	1.01×10^{-4}	2.81×10^3	0.0930	0.2150	-0.1363
Averaged[a]	5.668	0.2117	9.77×10^{-5}	2.60×10^3	0.4016	0.2064	-0.1251
Smoothed	343.840	0.00349	4.07×10^{-5}	1.03×10^2	0.5154	0.2013	0.8404

[a] FLOWTHRU-determined percentage of data to process (= 50%).
Transport distance $L = 1.20$ m.
Discharge flow $Q = 0.024$ m^3 h^{-1}.
Background concentration $\overline{C}_b = 0.160$ ppm (subtracted from data file).

5.2.1. Turner Designs Data File Creek.prn

The data file Creek.prn was developed from a field study in which the Model 10-AU-005 was set to log data every 30 min with concentrations reported in ppb. Data downloading was initiated 13 days after tracer injection and a follow-up data downloading approximately one day later. The first instance of data downloading resulted in a time break of 46 min, 27 s, which translates into a 16 min, 27 s, logger shutdown time during which logged data were downloaded (actual data transfer is generally much more rapid than 16 min, but minor difficulties can cause extended time delays).

Although an ~16.5 min loss of time is relatively insignificant for a tracer test lasting >13 days, it can be significant for tracer tests of a shorter duration. Alternatively, time breaks of a much greater duration, such as would occur during a power outage, can be very significant for a tracer test of this duration. Therefore, it is critical that any analysis of the logged data consider and properly compensate for inopportune time breaks in the logged data file.

Figure 39 is a plot of the time-concentration data file in decimal days using all the data. An arrow depicting the location of the lost time (~16.5 min) is also shown in Figure 39. Because there are so much data shown in Figure 39 and because the missing time is so insignificant relative to the overall duration of the tracer test, it is not visually possible to distinguish where the missing time exactly occurs.

Figure 40 is a plot of the time-concentration data file in decimal days using <10% of the data (FLOWTHRU-determined percentage to process). The arrows shown in Figure 40 now more clearly indicate the location of missing time relative to the recorded data. From Figure 40 (and less so from Figure 39) it may be discerned that the break in time recording occurred slightly after 13 days since the time of injection. Also more apparent is the relative insignificance of the missing data in this particular instance. (Note: The arrows depicted in Figures 39 and 40 are shown here only for illustration purposes and are not part of the FLOWTHRU package.)

5.3. PROCESSING VERY COMPLEX DATA FILES

Long-term tracer tests can result in some very complex data files because of (1) acquisition of a large amount of logged data, (2) numerous time breaks in the data reflecting frequent interruptions in data logging to download data, (3) significant loss of data as a result of a power outage or power surge causing an interruption in logger operation, or (4) some combination of any of the three previously identified issues causing complexity.
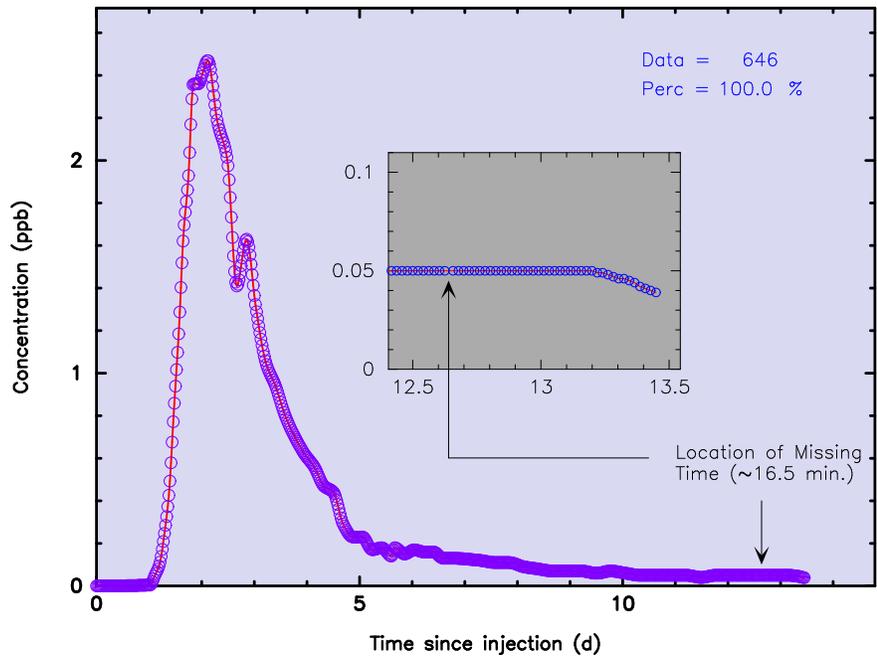
Figure 39. Decimal time-concentration data file for the Creek.prn data file developed from a 2 km tracer test (100% of the data shown). Note arrow indicating the location of missing time.
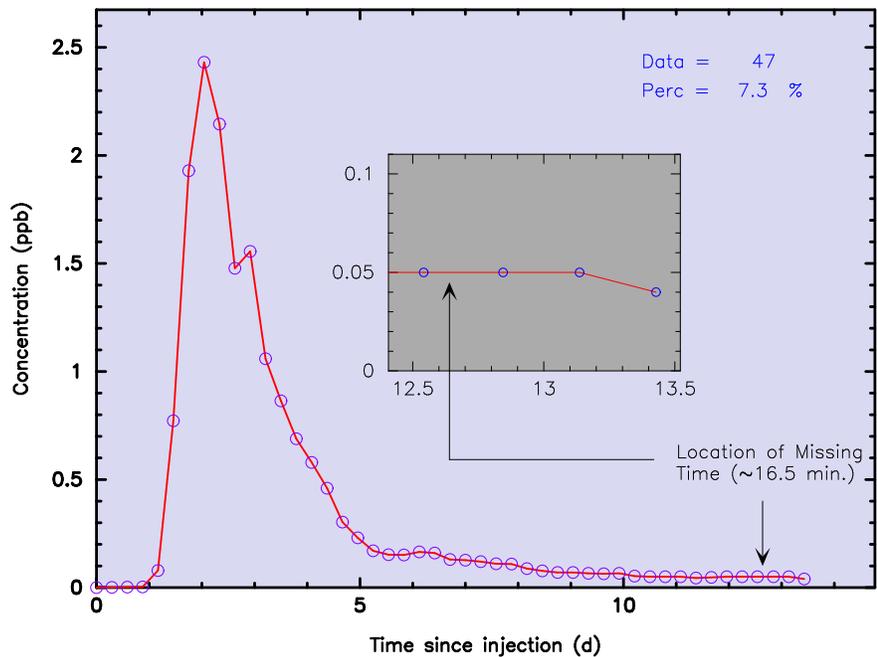
Figure 40. Decimal time-concentration data file for the Creek.prn data file developed from a 2 km tracer test (<10% of the data shown). Note arrow indicating the location of missing time. Also note expanded graph inset with missing time more prominently depicted.

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5.3.1.   Turner Designs Data File Fluor_time.prn

The data file Fluor_time.prn was developed from a field study in which the Model 10-AU-005 was set to log data every 10 min with concentrations reported in $\mu g\, L^{-1}$. Data downloading occurred several times after tracer injection, with numerous time interruptions and 19,995 total instrument-logged data. Although not all instances of data downloading resulted in significant logger interruptions during which logged data were downloaded, several of them did result in fairly long time breaks (e.g., >20 min).

Figure 41 is a plot of the time-concentration data file in decimal days using all the data; the BTC shown in Figure 41 suggests no time breaks. This is because the very large amount of data collected over a fairly long period coupled with the fact that the time breaks were limited to $\sim 20 - 30$ min tend to minimize the expected negative effect of missing time-concentration data. In addition, FLOWTHRU further realistically minimizes the expected negative effect by properly counting the lost time and adjusting the BTC.

The very large amount of data depicted in Figure 41 makes it very difficult to discern particular features of the Fluor_time.prn data set. This difficulty may be overcome by instructing FLOWTHRU to process only a portion of the data. Figure 42 is a plot of the time-concentration data file in decimal days with FLOWTHRU set for processing the data for each single day (i.e., 0.71% of the data processed).

Processing may be further enhanced by processing still less data than occur every day. For example, Figure 43 is a plot of the time-concentration data file in decimal days with FLOWTHRU set for processing the data every two days (i.e., 0.36% of the data processed). Figure 44 is a plot of the time-concentration data file in decimal days with FLOWTHRU set for processing the data every five days (i.e., 0.15% of the data processed), and Figure 45 is a plot of the time-concentration data file in decimal days with FLOWTHRU set for processing the data every 10 days (i.e., 0.075% of the data processed). Not readily apparent in Figures 42–45 is that counting past selected time values at a set frequency will usually result in the last one or more data points not being counted because it (they) does not match the chosen time spacing Δs_t. FLOWTHRU is designed to recognize this situation and process the last uncounted data points even though the Δs_t is not maintained.

Figure 46 is a plot of the time-concentration data file in decimal days with FLOWTHRU set to process just 2% of the data. Instructing FLOWTHRU of the percent of data to process may be more desirable in many instances. Figure 46 shows a much more useful amount of processed data (i.e., 400 data points) while not having to deal with the entire amount of data (i.e., 19,995 data points), which may overwhelm memory limitations set in some computer modeling programs.
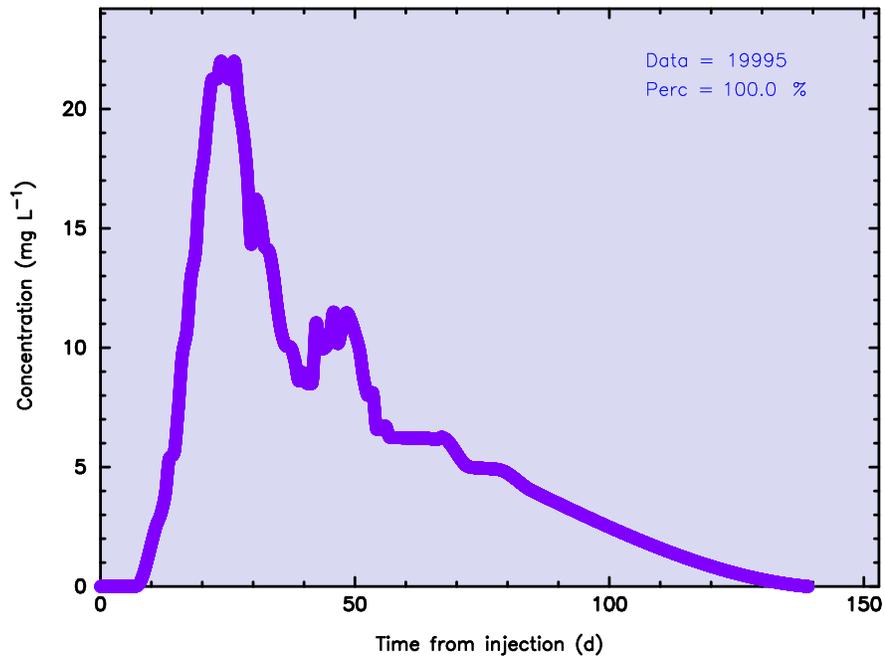
Figure 41. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test (100% of the data shown).
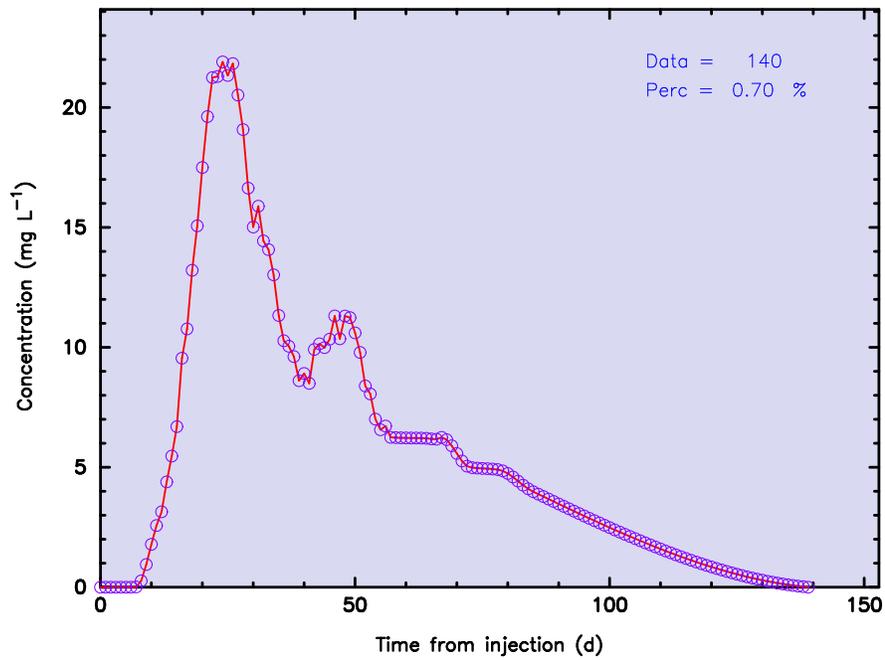
Figure 42. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test where data are processed for each day (0.71% of the data shown).
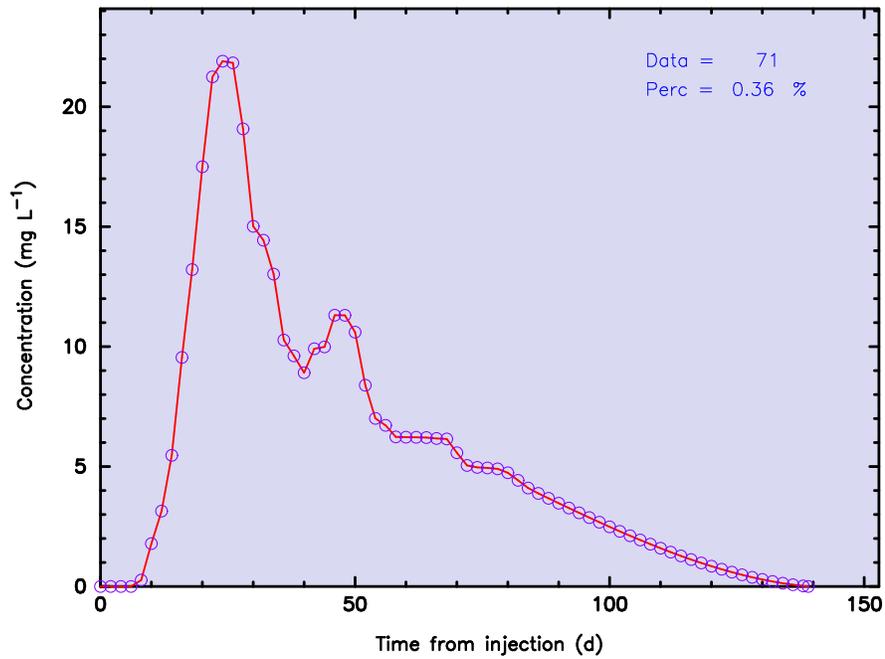
Figure 43. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test where data are processed for every other day (0.36% of the data shown).
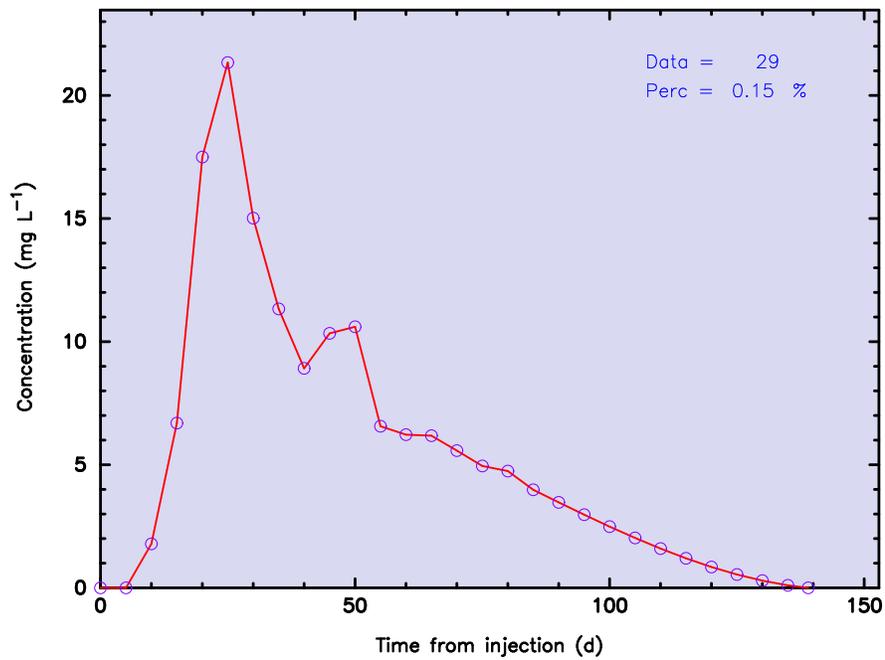
Figure 44. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test where data are processed for every fifth day (0.15% of the data shown).
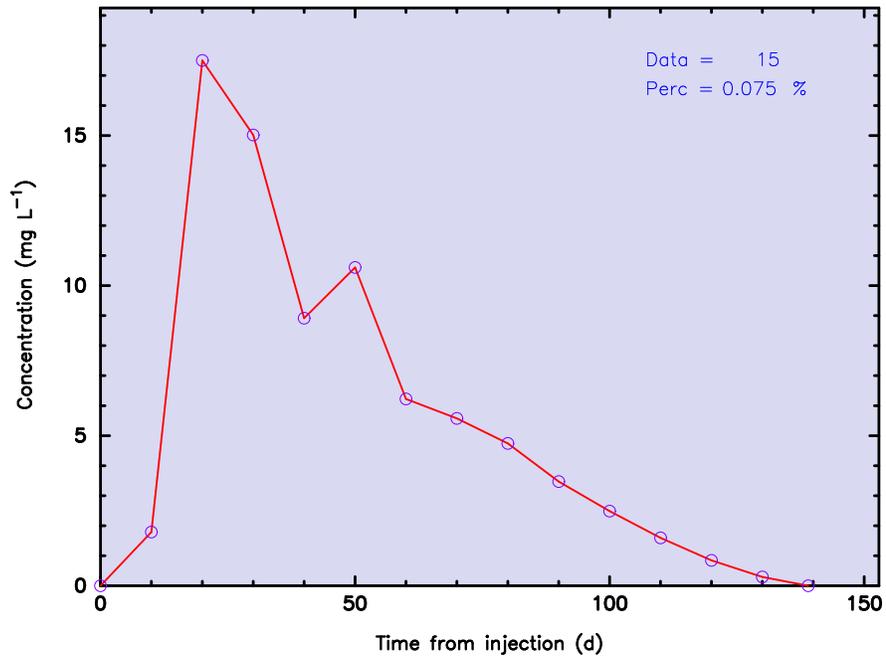
Figure 45. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test where data are processed for every tenth day (0.075% of the data shown).
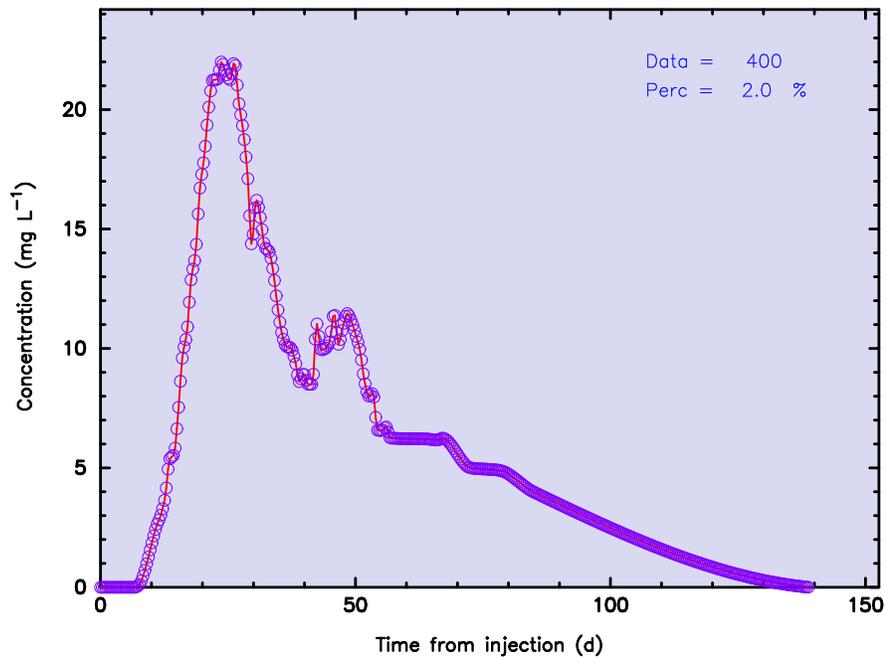
Figure 46. Decimal time-concentration data file for the Fluor_time.prn data file developed from a 5 km tracer test and set for 2% of the data as shown.

5.3.2.   Turner Designs Data File Break.prn

The data file Break.prn was developed from a field study in which the Model 10-AU-005 was set to log data every 10 min with concentrations reported in $\mu g\,L^{-1}$. This data file was modified to simulate the effect of an extremely large time break in the logged data file. Data downloading occurred several times after tracer injection. The first 10 instances of data downloading resulted in relatively insignificant logger interruptions during which logged data were downloaded. However, ~33 days after tracer injection, a power outage disrupted data logging. Due to the length of time of this experiment, an equipment check was not performed until the next planned date for data downloading (~58 days after tracer injection). The effect of logger shutdown was the loss of ~24.7 days of tracer data at a critical time during the tracer experiment.

Unlike the minor time break in the Creek.prn data set, the major time break in the Break.prn file is very significant because so much data were lost and because it occurred just after(?) peak tracer arrival (realistically, it is impossible to know the full effect of the missing data; it is entirely possible that peak recovery was actually missed). However, the data that were acquired still need to be properly assessed, which requires that the lost time be properly taken into account and the subsequent data properly adjusted for the lost time.

Figure 47 is a plot of the time-concentration data file in decimal days using all the data. Arrows depicting the location of the lost time (~25.5 days) are shown in Figure 47. Because there are so much lost data in the Break.prn file, a huge break in time is shown in Figure 47.

Figure 48 is a plot of the time-concentration data file in decimal days for 1.5% of the total logged time-concentration data (FLOWTHRU-determined percentage). The arrows shown on Figure 48 more clearly indicates the location of missing time relative to the recorded data. From Figure 48 (and equally so from Figure 47) it may be discerned that the break in time recording occurred slightly after 30 days since the time of injection. (Note: The arrows depicted in Figures 47 and 48 are shown only for illustration purposes and are not part of the FLOWTHRU package.)

5.3.3.   Turner Designs Data File 03g158.prn

The data file 03g158.prn was developed from a field study in which the Model 10-AU-005 developed by Michaël Verrault (Les Laboratoires SL, Chicoutimi, Québec) was set to log data every 30 min with concentrations listed in $\mu g\,L^{-1}$. The test consisted of an injection of 0.457 kg of dye over one hour on November 11, 2003, beginning at 1320 hours.

Unfortunately, almost immediately after the test was initiated, a power failure and subsequent
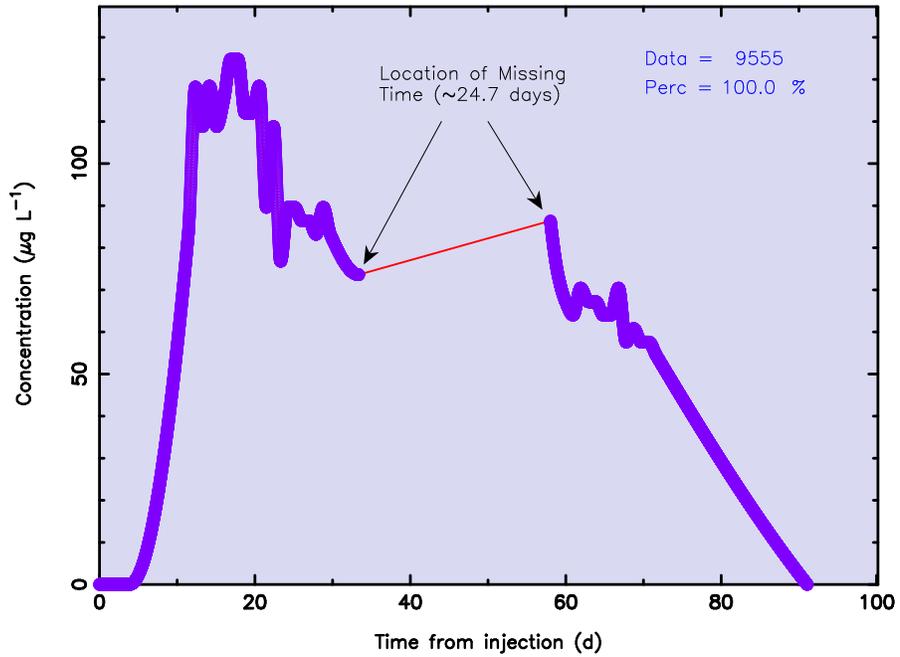
Figure 47. Decimal time-concentration data file for the Break.prn data file developed from a 5 km tracer test (100% of the data shown). Note arrows indicating the location of missing time.
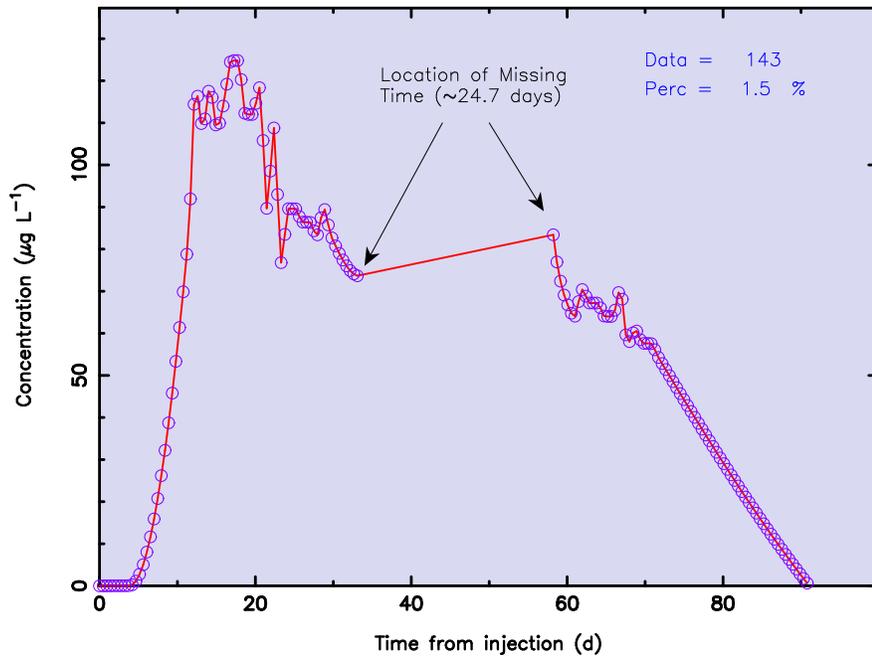

Figure 48. Decimal time-concentration data file for the Break.prn data file developed from a 5 km tracer test (1.5% of the total data shown). Note arrows indicating the location of missing time.

power surge severely damaged an internal NVRAM memory chip in the Model 10-AU-005, necessitating replacement. The time delay caused by determining the source of the instrument's internal problem, ordering a new NAVRAM chip, and installing the chip was significant. The fluorometer was repaired and restarted on November 24, 2003, at 1158 hours resulting in a total down time that exceeded 21 days. However, tracer migration was sufficiently slow such that a large portion of the tracer was still detected and logged by the fluorometer.

Figure 49 is a plot of all the logged data, Figure 50 is a plot of ∼50% of the data (50% chosen by "user"), and Figure 51 is a plot of ∼11% of the data (percentage determined by computer).

Arrows depicting the location of the lost time (13 days) are shown in Figures 49–51. Because there are so much lost data in 03g158.prn, a huge break in time is shown immediately after the start of the tracer test in Figures 49–51.

Figure 51 illustrates a potentially serious problem that occurs when the percentage of data used in processing FLOWTHRU is too small. Comparing Figure 51 with Figures 49 and 50 shows that a significant amount of important data around the "peak concentration" where concentration values were fluctuating were not processed by FLOWTHRU when only 11% of the data was processed. In this particular instance the low percentage of data display is not a serious factor in terms of BTC analysis (ignoring the data missing as a result of instrument failure). Comparing Figures 49, 50, and 51 shows that even though a selection of 11% of data was used in processing Figure 51, the unprocessed data lie almost directly below the peak concentration value.

It will also be noted that the last data point in the data file 03g158.prn was also not processed by FLOWTHRU when only 10% of the data were processed. As a result, the dropoff in concentration for the final logged data value is not apparent from Figure 49. Again, this unprocessed data point lies almost directly below the immediately prior data, so the effect of not processing this last data value is not serious in terms of time-of-travel analyses. However, the user will need to check FLOWTHRU output files carefully to ensure that all data that should have been processed were actually processed.

5.3.3.1. *Effect of Data Point Deletion on File 03g158.prn.*   The failure of the NAVRAM chip in the fluorometer and the eventual restarting of the fluorometer are suspected of also having resulted in some anomalous data points. Specifically, the second data point (12.9434,0.086) is suspect and the very last data point (21.8634,0.123) is questionable (see Figures 49–51).

Using the interactive feature of FLOWTHRU to select these two data points resulted in the deletion of these data points. Figure 52 is a plot of the "full" data set minus the two deleted data points. Comparing Figure 52 with Figure 49 shows a reduction in the number of data points
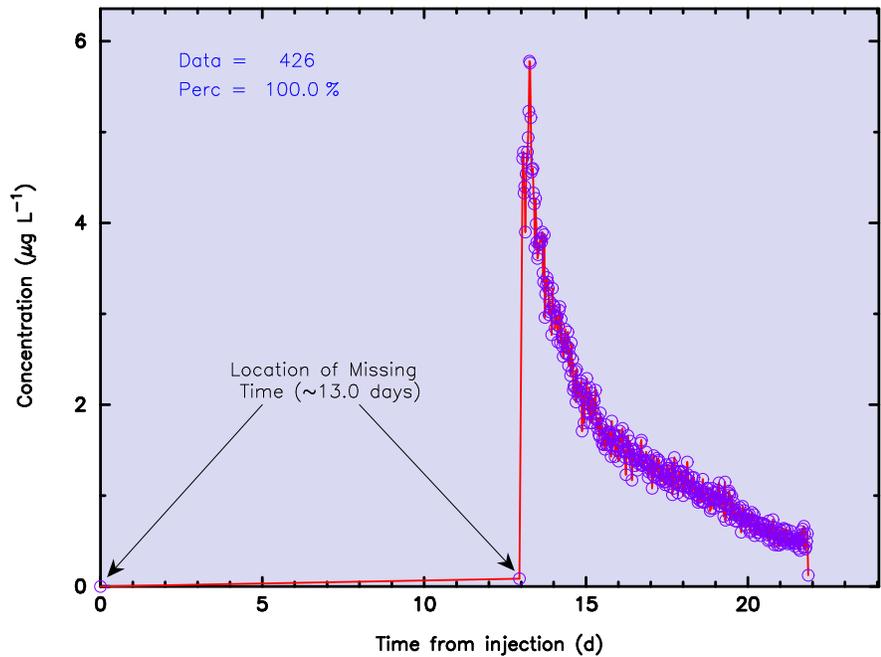
Figure 49. Decimal time-concentration data file for the 03g158.prn data file developed from a tracer test (100% of the data shown). Note arrows indicating the location of missing time.
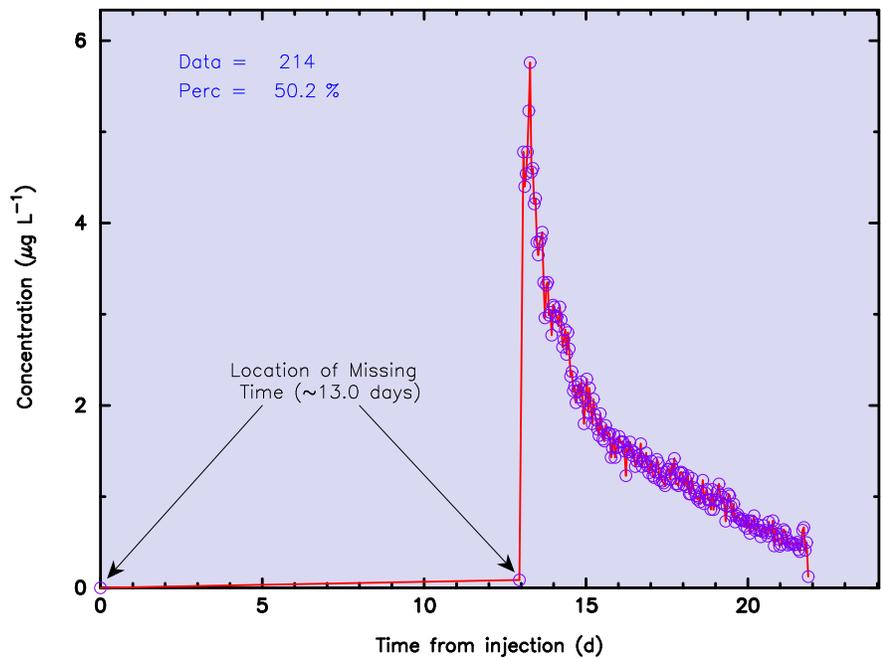
Figure 50. Decimal time-concentration data file for the 03g158.prn data file developed from a tracer test (~50% of the data shown). Note arrows indicating the location of missing time.
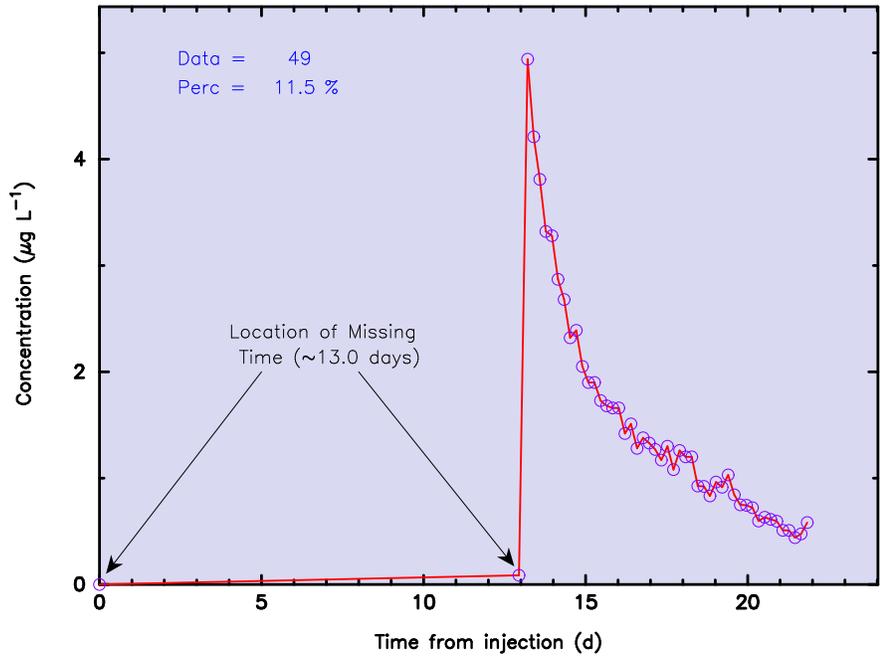
Figure 51. Decimal time-concentration data file for the 03g158.prn data file developed from a tracer test (~11% of the data shown). Note arrows indicating the location of missing time.
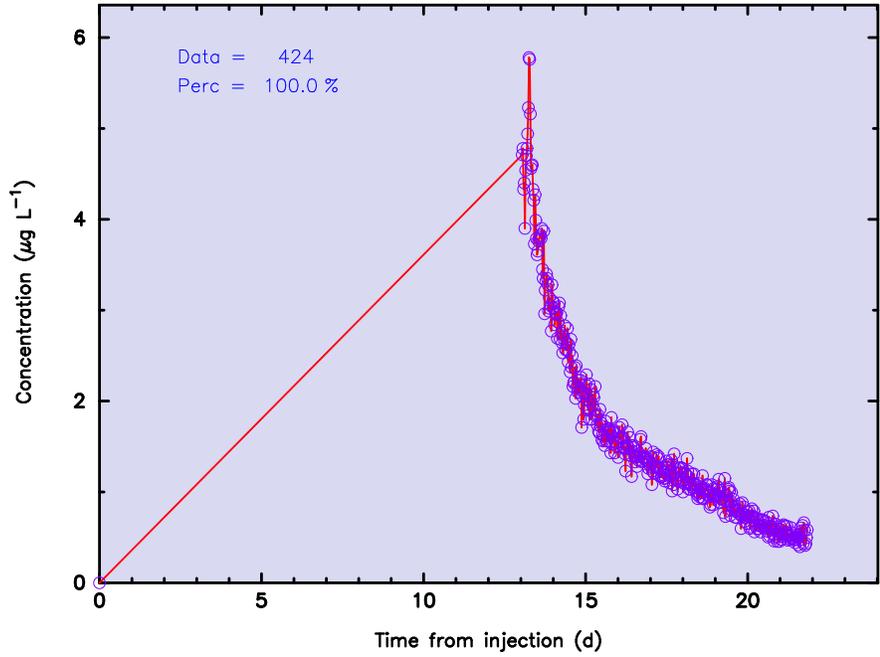
Figure 52. Decimal time-concentration data file for the 03g158.prn data file in which the second (12.9434,0.086) and last (21.8634,0.123) data points have been deleted using FLOWTHRU.

processed but those that were processed were counted as 100% complete.

6. SUMMARY

Continuous recording of dye fluorescence using field fluorometers at selected sampling sites is a commonly applied measurement technique. Unfortunately, the general form of data logged by a Turner Designs Model 10-AU-005 and downloaded using the Turner Designs IDL_1B1 program does not readily lend itself to rapid and easy analysis. A new computer program, FLOWTHRU, efficiently reads the data logged by the Model 10-AU-005, converts the data to decimal time, and plots the data directly to a computer monitor, which allows trends in the data to be quickly discerned. Use of FLOWTHRU on Model 10-AU-005 logged data is a useful complement to the IDL_1B1 program and facilitates data analysis. Useful features of the program FLOWTHRU include:

1. the ability to read-in a simple process control data file or interactive responses from the user;

2. extensive error-checking and error-correction routine to facilitate data processing;

3. conversion of logged date and time to decimal days, hours, minutes, seconds;

4. processing of measured data, a percentage of the data set by the user or by FLOWTHRU, daily or hourly data, block averaged data, or smoothed data using a moving average;

5. listing and file creation of the converted time-concentration data file for use in other modeling packages;

6. listing and file creation of background time-concentration data and water temperature data;

7. date and time adjustments to account for lost time due to instrument malfunction or other circumstance; and

8. graphical and publication-quality PostScript plot generation of FLOWTHRU, results allowing for real-time evaluation of the tracer data.

This program greatly enhances the capabilities of the Turner Designs Model 10-AU-005 field filter fluorometer when used in the continuous flow-through mode. It should lead to greater reliance on continuous monitoring during dye-tracing experiments in the future because of the vastly superior amount of data collected, quality (accuracy and precision) of the data collected, and ease with which the data may be evaluated.

APPENDIX I

TABLE OF ERRORS RESULTING FROM A COMPARISON OF MEASURED CONCENTRATIONS VERSUS SMOOTHED CONCENTRATIONS

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
1	0.0000	0.160	0.094	0.066	0.413
2	0.0167	0.160	0.103	0.057	0.356
3	0.0334	0.160	0.112	0.048	0.300
4	0.0500	0.160	0.121	0.039	0.243
5	0.0667	0.160	0.130	0.030	0.187
6	0.0834	0.160	0.139	0.021	0.130
7	0.1000	0.164	0.148	0.016	0.096
8	0.1167	0.189	0.157	0.032	0.168
9	0.1334	0.238	0.166	0.072	0.301
10	0.1500	0.250	0.175	0.075	0.298
11	0.1667	0.228	0.184	0.044	0.191
12	0.1834	0.208	0.189	0.019	0.092
13	0.2000	0.199	0.192	0.007	0.033
14	0.2167	0.189	0.195	−0.006	−0.032
15	0.2334	0.172	0.196	−0.024	−0.140
16	0.2500	0.163	0.196	−0.033	−0.205
17	0.2667	0.179	0.198	−0.019	−0.107
18	0.2834	0.203	0.202	0.001	0.007
19	0.3000	0.204	0.203	0.001	0.005
20	0.3167	0.190	0.199	−0.009	−0.045
21	0.3334	0.174	0.192	−0.018	−0.102
22	0.3500	0.164	0.186	−0.022	−0.134
23	0.3667	0.160	0.182	−0.022	−0.135
24	0.3834	0.160	0.178	−0.018	−0.113
25	0.4000	0.160	0.175	−0.015	−0.096
26	0.4167	0.160	0.174	−0.014	−0.089
27	0.4334	0.160	0.174	−0.014	−0.087
28	0.4500	0.160	0.172	−0.012	−0.077
29	0.4667	0.160	0.168	−0.008	−0.052
30	0.4834	0.159	0.164	−0.005	−0.033
31	0.5000	0.160	0.162	−0.002	−0.010
32	0.5167	0.162	0.160	0.002	0.010
33	0.5334	0.162	0.160	0.002	0.011

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
34	0.5500	0.162	0.160	0.002	0.010
35	0.5667	0.160	0.160	0.000	−0.003
36	0.5834	0.159	0.160	−0.001	−0.009
37	0.6000	0.159	0.160	−0.001	−0.008
38	0.6167	0.160	0.160	0.000	−0.002
39	0.6334	0.160	0.160	0.000	−0.002
40	0.6500	0.162	0.160	0.002	0.010
41	0.6667	0.160	0.161	−0.001	−0.003
42	0.6834	0.160	0.161	−0.001	−0.003
43	0.7000	0.160	0.160	0.000	−0.002
44	0.7167	0.160	0.160	0.000	−0.001
45	0.7334	0.160	0.160	0.000	0.000
46	0.7500	0.159	0.160	−0.001	−0.006
47	0.7667	0.160	0.160	0.000	0.000
48	0.7834	0.159	0.160	−0.001	−0.006
49	0.8000	0.158	0.160	−0.002	−0.012
50	0.8167	0.158	0.160	−0.002	−0.010
51	0.8334	0.159	0.159	0.000	−0.002
52	0.8500	0.160	0.159	0.001	0.004
53	0.8667	0.162	0.160	0.002	0.015
54	0.8834	0.162	0.160	0.002	0.014
55	0.9000	0.160	0.160	0.000	0.002
56	0.9167	0.160	0.160	0.000	0.002
57	0.9334	0.160	0.160	0.000	0.001
58	0.9500	0.162	0.160	0.002	0.012
59	0.9667	0.160	0.160	0.000	−0.001
60	0.9834	0.160	0.160	0.000	−0.002
61	1.0000	0.160	0.160	0.000	−0.003
62	1.0167	0.160	0.161	−0.001	−0.003
63	1.0334	0.160	0.161	−0.001	−0.003
64	1.0500	0.158	0.160	−0.002	−0.014
65	1.0667	0.158	0.160	−0.002	−0.012
66	1.0834	0.158	0.160	−0.002	−0.010
67	1.1000	0.160	0.160	0.000	0.002
68	1.1167	0.160	0.160	0.000	0.002
69	1.1334	0.160	0.159	0.001	0.003
70	1.1500	0.159	0.159	0.000	−0.002
71	1.1667	0.159	0.159	0.000	−0.002
72	1.1834	0.159	0.159	0.000	−0.001
73	1.2000	0.159	0.159	0.000	−0.001

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
74	1.2167	0.159	0.159	0.000	0.000
75	1.2334	0.159	0.159	0.000	−0.001
76	1.2500	0.159	0.159	0.000	−0.001
77	1.2667	0.159	0.159	0.000	−0.002
78	1.2834	0.159	0.159	0.000	−0.001
79	1.3000	0.159	0.159	0.000	−0.001
80	1.3167	0.160	0.159	0.001	0.006
81	1.3334	0.159	0.159	0.000	−0.001
82	1.3500	0.159	0.159	0.000	−0.001
83	1.3667	0.160	0.159	0.001	0.005
84	1.3834	0.160	0.159	0.001	0.005
85	1.4000	0.160	0.159	0.001	0.004
86	1.4167	0.160	0.159	0.001	0.003
87	1.4334	0.160	0.160	0.000	0.003
88	1.4500	0.160	0.160	0.000	0.002
89	1.4667	0.160	0.160	0.000	0.002
90	1.4834	0.160	0.160	0.000	0.001
91	1.5000	0.162	0.160	0.002	0.012
92	1.5167	0.163	0.160	0.003	0.016
93	1.5334	0.163	0.161	0.002	0.014
94	1.5500	0.162	0.161	0.001	0.007
95	1.5667	0.160	0.161	−0.001	−0.006
96	1.5834	0.160	0.161	−0.001	−0.006
97	1.6000	0.160	0.161	−0.001	−0.006
98	1.6167	0.159	0.161	−0.002	−0.011
99	1.6334	0.160	0.161	−0.001	−0.005
100	1.6500	0.160	0.161	−0.001	−0.005
101	1.6667	0.160	0.161	−0.001	−0.005
102	1.6834	0.159	0.161	−0.002	−0.010
103	1.7000	0.159	0.160	−0.001	−0.007
104	1.7167	0.162	0.160	0.002	0.012
105	1.7334	0.162	0.160	0.002	0.012
106	1.7500	0.160	0.160	0.000	−0.001
107	1.7667	0.160	0.160	0.000	−0.001
108	1.7834	0.160	0.160	0.000	−0.001
109	1.8000	0.162	0.160	0.002	0.010
110	1.8167	0.160	0.160	0.000	−0.002
111	1.8334	0.159	0.160	−0.001	−0.008
112	1.8500	0.160	0.160	0.000	−0.002
113	1.8667	0.160	0.160	0.000	−0.002

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
114	1.8834	0.159	0.160	−0.001	−0.009
115	1.9000	0.159	0.160	−0.001	−0.007
116	1.9167	0.160	0.160	0.000	0.001
117	1.9334	0.162	0.160	0.002	0.012
118	1.9500	0.162	0.160	0.002	0.011
119	1.9667	0.162	0.160	0.002	0.010
120	1.9834	0.162	0.160	0.002	0.010
121	2.0000	0.160	0.160	0.000	−0.003
122	2.0167	0.162	0.161	0.001	0.008
123	2.0334	0.162	0.161	0.001	0.007
124	2.0500	0.163	0.161	0.002	0.011
125	2.0667	0.165	0.162	0.003	0.020
126	2.0834	0.165	0.162	0.003	0.017
127	2.1000	0.165	0.163	0.002	0.014
128	2.1167	0.166	0.163	0.003	0.018
129	2.1334	0.168	0.164	0.004	0.026
130	2.1500	0.170	0.164	0.006	0.033
131	2.1667	0.170	0.165	0.005	0.029
132	2.1834	0.172	0.166	0.006	0.034
133	2.2000	0.173	0.167	0.006	0.034
134	2.2167	0.175	0.168	0.007	0.038
135	2.2334	0.178	0.170	0.008	0.046
136	2.2500	0.179	0.171	0.008	0.045
137	2.2667	0.179	0.172	0.007	0.038
138	2.2834	0.181	0.174	0.007	0.040
139	2.3000	0.182	0.175	0.007	0.037
140	2.3167	0.184	0.177	0.007	0.040
141	2.3334	0.187	0.178	0.009	0.047
142	2.3500	0.187	0.180	0.007	0.039
143	2.3667	0.187	0.181	0.006	0.032
144	2.3834	0.188	0.182	0.006	0.029
145	2.4000	0.190	0.184	0.006	0.033
146	2.4167	0.193	0.185	0.008	0.041
147	2.4334	0.194	0.187	0.007	0.038
148	2.4500	0.195	0.188	0.007	0.036
149	2.4667	0.195	0.189	0.006	0.029
150	2.4834	0.197	0.191	0.006	0.032
151	2.5000	0.200	0.192	0.008	0.040
152	2.5167	0.203	0.194	0.009	0.047
153	2.5334	0.206	0.195	0.011	0.052

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
154	2.5500	0.206	0.197	0.009	0.044
155	2.5667	0.208	0.199	0.009	0.044
156	2.5834	0.209	0.201	0.008	0.040
157	2.6000	0.209	0.202	0.007	0.033
158	2.6167	0.209	0.203	0.006	0.027
159	2.6334	0.209	0.205	0.004	0.021
160	2.6500	0.210	0.206	0.004	0.019
161	2.6667	0.209	0.207	0.002	0.009
162	2.6834	0.209	0.208	0.001	0.005
163	2.7000	0.211	0.209	0.002	0.011
164	2.7167	0.212	0.209	0.003	0.013
165	2.7334	0.214	0.210	0.004	0.019
166	2.7500	0.212	0.210	0.002	0.008
167	2.7667	0.212	0.211	0.001	0.007
168	2.7834	0.214	0.211	0.003	0.014
169	2.8000	0.211	0.211	0.000	−0.001
170	2.8167	0.210	0.211	−0.001	−0.006
171	2.8334	0.210	0.211	−0.001	−0.006
172	2.8500	0.211	0.211	0.000	−0.002
173	2.8667	0.211	0.212	−0.001	−0.003
174	2.8834	0.209	0.211	−0.002	−0.012
175	2.9000	0.209	0.211	−0.002	−0.010
176	2.9167	0.209	0.211	−0.002	−0.008
177	2.9334	0.209	0.210	−0.001	−0.007
178	2.9500	0.209	0.210	−0.001	−0.006
179	2.9667	0.207	0.210	−0.003	−0.012
180	2.9834	0.204	0.209	−0.005	−0.024
181	3.0000	0.204	0.208	−0.004	−0.021
182	3.0167	0.203	0.208	−0.005	−0.023
183	3.0334	0.203	0.207	−0.004	−0.020
184	3.0500	0.202	0.206	−0.004	−0.021
185	3.0667	0.200	0.205	−0.005	−0.027
186	3.0834	0.199	0.204	−0.005	−0.027
187	3.1000	0.196	0.203	−0.007	−0.037
188	3.1167	0.195	0.202	−0.007	−0.036
189	3.1334	0.196	0.201	−0.005	−0.025
190	3.1500	0.195	0.200	−0.005	−0.024
191	3.1667	0.194	0.199	−0.005	−0.025
192	3.1834	0.193	0.198	−0.005	−0.025
193	3.2000	0.189	0.197	−0.008	−0.040

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
194	3.2167	0.189	0.195	−0.006	−0.033
195	3.2334	0.189	0.194	−0.005	−0.027
196	3.2500	0.187	0.193	−0.006	−0.032
197	3.2667	0.187	0.192	−0.005	−0.026
198	3.2834	0.187	0.191	−0.004	−0.021
199	3.3000	0.186	0.190	−0.004	−0.022
200	3.3167	0.186	0.189	−0.003	−0.018
201	3.3334	0.186	0.188	−0.002	−0.013
202	3.3500	0.185	0.188	−0.003	−0.014
203	3.3667	0.181	0.187	−0.006	−0.031
204	3.3834	0.180	0.186	−0.006	−0.032
205	3.4000	0.179	0.185	−0.006	−0.033
206	3.4167	0.179	0.184	−0.005	−0.027
207	3.4334	0.177	0.183	−0.006	−0.034
208	3.4500	0.175	0.182	−0.007	−0.039
209	3.4667	0.175	0.181	−0.006	−0.033
210	3.4834	0.175	0.180	−0.005	−0.028
211	3.5000	0.173	0.179	−0.006	−0.033
212	3.5167	0.173	0.177	−0.004	−0.026
213	3.5334	0.172	0.176	−0.004	−0.025
214	3.5500	0.170	0.175	−0.005	−0.031
215	3.5667	0.170	0.174	−0.004	−0.026
216	3.5834	0.170	0.174	−0.004	−0.021
217	3.6000	0.170	0.173	−0.003	−0.016
218	3.6167	0.170	0.172	−0.002	−0.012
219	3.6334	0.170	0.172	−0.002	−0.010
220	3.6500	0.170	0.171	−0.001	−0.007
221	3.6667	0.170	0.171	−0.001	−0.004
222	3.6834	0.167	0.170	−0.003	−0.019
223	3.7000	0.166	0.170	−0.004	−0.021
224	3.7167	0.167	0.169	−0.002	−0.013
225	3.7334	0.166	0.169	−0.003	−0.016
226	3.7500	0.165	0.168	−0.003	−0.020
227	3.7667	0.165	0.168	−0.003	−0.017
228	3.7834	0.165	0.167	−0.002	−0.014
229	3.8000	0.165	0.167	−0.002	−0.012
230	3.8167	0.165	0.166	−0.001	−0.009
231	3.8334	0.165	0.166	−0.001	−0.006
232	3.8500	0.165	0.166	−0.001	−0.003
233	3.8667	0.165	0.165	0.000	−0.002

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
234	3.8834	0.165	0.165	0.000	−0.002
235	3.9000	0.165	0.165	0.000	−0.001
236	3.9167	0.165	0.165	0.000	0.000
237	3.9334	0.165	0.165	0.000	0.000
238	3.9500	0.165	0.165	0.000	0.000
239	3.9667	0.165	0.165	0.000	0.000
240	3.9834	0.165	0.165	0.000	0.000
241	4.0000	0.164	0.165	−0.001	−0.006
242	4.0167	0.163	0.165	−0.002	−0.011
243	4.0334	0.164	0.165	−0.001	−0.004
244	4.0500	0.163	0.164	−0.001	−0.009
245	4.0667	0.160	0.164	−0.004	−0.025
246	4.0834	0.162	0.164	−0.002	−0.011
247	4.1000	0.162	0.163	−0.001	−0.009
248	4.1167	0.162	0.163	−0.001	−0.007
249	4.1334	0.160	0.163	−0.003	−0.017
250	4.1500	0.160	0.162	−0.002	−0.014
251	4.1667	0.160	0.162	−0.002	−0.011
252	4.1834	0.162	0.162	0.000	0.002
253	4.2000	0.164	0.162	0.002	0.014
254	4.2167	0.164	0.162	0.002	0.014
255	4.2334	0.164	0.162	0.002	0.013
256	4.2500	0.163	0.162	0.001	0.006
257	4.2667	0.163	0.162	0.001	0.005
258	4.2834	0.163	0.162	0.001	0.004
259	4.3000	0.164	0.162	0.002	0.009
260	4.3167	0.162	0.163	−0.001	−0.004
261	4.3334	0.159	0.163	−0.004	−0.022
262	4.3500	0.158	0.162	−0.004	−0.028
263	4.3667	0.160	0.162	−0.002	−0.014
264	4.3834	0.160	0.162	−0.002	−0.011
265	4.4000	0.160	0.161	−0.001	−0.009
266	4.4167	0.160	0.161	−0.001	−0.007
267	4.4334	0.162	0.161	0.001	0.006
268	4.4500	0.162	0.161	0.001	0.007
269	4.4667	0.160	0.161	−0.001	−0.004
270	4.4834	0.160	0.160	0.000	−0.002
271	4.5000	0.160	0.160	0.000	−0.001
272	4.5167	0.159	0.160	−0.001	−0.007
273	4.5334	0.158	0.160	−0.002	−0.013

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
274	4.5500	0.159	0.160	−0.001	−0.006
275	4.5667	0.160	0.160	0.000	0.000
276	4.5834	0.160	0.160	0.000	0.000
277	4.6000	0.160	0.160	0.000	0.000
278	4.6167	0.160	0.160	0.000	0.001
279	4.6334	0.159	0.160	−0.001	−0.003
280	4.6500	0.159	0.159	0.000	−0.003
281	4.6667	0.158	0.159	−0.001	−0.008
282	4.6834	0.158	0.159	−0.001	−0.007
283	4.7000	0.159	0.159	0.000	−0.001
284	4.7167	0.159	0.159	0.000	−0.001
285	4.7334	0.158	0.159	−0.001	−0.007
286	4.7500	0.158	0.159	−0.001	−0.006
287	4.7667	0.159	0.159	0.000	0.001
288	4.7834	0.159	0.159	0.000	0.002
289	4.8000	0.160	0.159	0.001	0.008
290	4.8167	0.160	0.159	0.001	0.007
291	4.8334	0.160	0.159	0.001	0.007
292	4.8500	0.162	0.159	0.003	0.017
293	4.8667	0.160	0.159	0.001	0.003
294	4.8834	0.159	0.159	0.000	−0.003
295	4.9000	0.160	0.160	0.000	0.003
296	4.9167	0.160	0.160	0.000	0.002
297	4.9334	0.159	0.160	−0.001	−0.005
298	4.9500	0.158	0.160	−0.002	−0.011
299	4.9667	0.158	0.160	−0.002	−0.010
300	4.9834	0.159	0.160	−0.001	−0.003
301	5.0000	0.159	0.159	0.000	−0.003
302	5.0167	0.160	0.159	0.001	0.003
303	5.0334	0.160	0.159	0.001	0.005
304	5.0500	0.160	0.159	0.001	0.005
305	5.0667	0.159	0.159	0.000	−0.002
306	5.0834	0.159	0.159	0.000	−0.001
307	5.1000	0.159	0.159	0.000	−0.001
308	5.1167	0.160	0.159	0.001	0.005
309	5.1334	0.162	0.160	0.002	0.015
310	5.1500	0.162	0.160	0.002	0.013
311	5.1667	0.160	0.160	0.000	0.000
312	5.1834	0.160	0.160	0.000	−0.001
313	5.2000	0.160	0.160	0.000	−0.001

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
314	5.2167	0.160	0.160	0.000	−0.001
315	5.2334	0.159	0.160	−0.001	−0.006
316	5.2500	0.159	0.160	−0.001	−0.006
317	5.2667	0.160	0.160	0.000	−0.001
318	5.2834	0.162	0.160	0.002	0.010
319	5.3000	0.162	0.161	0.001	0.009
320	5.3167	0.162	0.161	0.001	0.009
321	5.3334	0.160	0.160	0.000	−0.002
322	5.3500	0.160	0.160	0.000	−0.002
323	5.3667	0.160	0.160	0.000	−0.002
324	5.3834	0.162	0.161	0.001	0.009
325	5.4000	0.162	0.161	0.001	0.008
326	5.4167	0.162	0.161	0.001	0.006
327	5.4334	0.162	0.161	0.001	0.004
328	5.4500	0.160	0.161	−0.001	−0.008
329	5.4667	0.160	0.161	−0.001	−0.007
330	5.4834	0.162	0.161	0.001	0.006
331	5.5000	0.160	0.161	−0.001	−0.006
332	5.5167	0.160	0.161	−0.001	−0.006
333	5.5334	0.162	0.161	0.001	0.006
334	5.5500	0.162	0.161	0.001	0.004
335	5.5667	0.160	0.161	−0.001	−0.007
336	5.5834	0.160	0.161	−0.001	−0.006
337	5.6000	0.160	0.161	−0.001	−0.005
338	5.6167	0.160	0.161	−0.001	−0.003
339	5.6334	0.160	0.161	−0.001	−0.003
340	5.6500	0.159	0.160	−0.001	−0.009
341	5.6667	0.159	0.160	−0.001	−0.007
342	5.6834	0.158	0.160	−0.002	−0.013
343	5.7000	0.158	0.160	−0.002	−0.012
344	5.7167	0.158	0.159	−0.001	−0.009
345	5.7334	0.158	0.159	−0.001	−0.007
346	5.7500	0.159	0.159	0.000	0.000
347	5.7667	0.160	0.159	0.001	0.006
348	5.7834	0.162	0.159	0.003	0.017
349	5.8000	0.159	0.159	0.000	−0.001
350	5.8167	0.158	0.159	−0.001	−0.006
351	5.8334	0.159	0.159	0.000	0.001
352	5.8500	0.159	0.159	0.000	0.001
353	5.8667	0.158	0.159	−0.001	−0.006

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
354	5.8834	0.159	0.159	0.000	0.000
355	5.9000	0.160	0.159	0.001	0.005
356	5.9167	0.160	0.159	0.001	0.004
357	5.9334	0.160	0.159	0.001	0.003
358	5.9500	0.159	0.159	0.000	−0.002
359	5.9667	0.160	0.159	0.001	0.005
360	5.9834	0.162	0.159	0.003	0.016
361	6.0000	0.162	0.160	0.002	0.013
362	6.0167	0.160	0.160	0.000	0.001
363	6.0334	0.159	0.160	−0.001	−0.006
364	6.0500	0.159	0.160	−0.001	−0.006
365	6.0667	0.159	0.160	−0.001	−0.006
366	6.0834	0.159	0.160	−0.001	−0.006
367	6.1000	0.160	0.160	0.000	0.001
368	6.1167	0.160	0.160	0.000	0.001
369	6.1334	0.160	0.160	0.000	0.000
370	6.1500	0.160	0.160	0.000	0.000
371	6.1667	0.159	0.160	−0.001	−0.005
372	6.1834	0.159	0.159	0.000	−0.003
373	6.2000	0.159	0.159	0.000	−0.002
374	6.2167	0.160	0.159	0.001	0.003
375	6.2334	0.159	0.159	0.000	−0.003
376	6.2500	0.159	0.159	0.000	−0.003
377	6.2667	0.160	0.160	0.000	0.003
378	6.2834	0.160	0.160	0.000	0.003
379	6.3000	0.160	0.160	0.000	0.003
380	6.3167	0.160	0.160	0.000	0.003
381	6.3334	0.160	0.160	0.000	0.003
382	6.3500	0.159	0.160	−0.001	−0.003
383	6.3667	0.158	0.159	−0.001	−0.009
384	6.3834	0.158	0.159	−0.001	−0.009
385	6.4000	0.159	0.159	0.000	−0.002
386	6.4167	0.159	0.159	0.000	−0.002
387	6.4334	0.159	0.159	0.000	−0.002
388	6.4500	0.160	0.159	0.001	0.005
389	6.4667	0.160	0.159	0.001	0.005
390	6.4834	0.160	0.159	0.001	0.005
391	6.5000	0.160	0.159	0.001	0.005
392	6.5167	0.159	0.159	0.000	−0.001
393	6.5334	0.159	0.159	0.000	−0.001

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
394	6.5500	0.160	0.159	0.001	0.004
395	6.5667	0.160	0.160	0.000	0.003
396	6.5834	0.158	0.159	−0.001	−0.009
397	6.6000	0.158	0.159	−0.001	−0.009
398	6.6167	0.159	0.159	0.000	−0.002
399	6.6334	0.160	0.159	0.001	0.004
400	6.6500	0.160	0.159	0.001	0.004
401	6.6667	0.160	0.159	0.001	0.004
402	6.6834	0.160	0.159	0.001	0.004
403	6.7000	0.159	0.159	0.000	−0.002
404	6.7167	0.159	0.159	0.000	−0.002
405	6.7334	0.159	0.159	0.000	−0.002
406	6.7500	0.159	0.159	0.000	−0.001
407	6.7667	0.159	0.159	0.000	−0.002
408	6.7834	0.160	0.159	0.001	0.003
409	6.8000	0.159	0.159	0.000	−0.003
410	6.8167	0.158	0.159	−0.001	−0.008
411	6.8334	0.159	0.159	0.000	−0.001
412	6.8500	0.158	0.159	−0.001	−0.006
413	6.8667	0.158	0.159	−0.001	−0.005
414	6.8834	0.158	0.159	−0.001	−0.005
415	6.9000	0.158	0.159	−0.001	−0.004
416	6.9167	0.159	0.159	0.000	0.002
417	6.9334	0.159	0.159	0.000	0.002
418	6.9500	0.160	0.159	0.001	0.008
419	6.9667	0.160	0.159	0.001	0.008
420	6.9834	0.160	0.159	0.001	0.007
421	7.0000	0.160	0.159	0.001	0.006
422	7.0167	0.162	0.159	0.003	0.017
423	7.0334	0.160	0.159	0.001	0.003
424	7.0500	0.162	0.160	0.002	0.013
425	7.0667	0.163	0.160	0.003	0.017
426	7.0834	0.162	0.161	0.001	0.008
427	7.1000	0.159	0.161	−0.002	−0.010
428	7.1167	0.159	0.161	−0.002	−0.010
429	7.1334	0.160	0.161	−0.001	−0.004
430	7.1500	0.160	0.161	−0.001	−0.004
431	7.1667	0.160	0.161	−0.001	−0.004
432	7.1834	0.160	0.161	−0.001	−0.004
433	7.2000	0.160	0.160	0.000	−0.003

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
434	7.2167	0.160	0.160	0.000	−0.003
435	7.2334	0.160	0.160	0.000	−0.002
436	7.2500	0.160	0.160	0.000	0.000
437	7.2667	0.160	0.160	0.000	0.001
438	7.2834	0.160	0.160	0.000	0.001
439	7.3000	0.160	0.160	0.000	0.000
440	7.3167	0.160	0.160	0.000	0.000
441	7.3334	0.159	0.160	−0.001	−0.006
442	7.3500	0.159	0.160	−0.001	−0.005
443	7.3667	0.159	0.160	−0.001	−0.005
444	7.3834	0.160	0.160	0.000	0.002
445	7.4000	0.160	0.160	0.000	0.002
446	7.4167	0.160	0.160	0.000	0.002
447	7.4334	0.160	0.160	0.000	0.002
448	7.4500	0.160	0.160	0.000	0.002
449	7.4667	0.160	0.160	0.000	0.002
450	7.4834	0.160	0.160	0.000	0.002
451	7.5000	0.160	0.160	0.000	0.002
452	7.5167	0.160	0.160	0.000	0.001
453	7.5334	0.159	0.160	−0.001	−0.005
454	7.5500	0.159	0.160	−0.001	−0.005
455	7.5667	0.159	0.160	−0.001	−0.005
456	7.5834	0.159	0.160	−0.001	−0.004
457	7.6000	0.160	0.160	0.000	0.002
458	7.6167	0.160	0.160	0.000	0.002
459	7.6334	0.159	0.160	−0.001	−0.003
460	7.6500	0.160	0.160	0.000	0.003
461	7.6667	0.160	0.160	0.000	0.003
462	7.6834	0.160	0.160	0.000	0.003
463	7.7000	0.160	0.160	0.000	0.003
464	7.7167	0.162	0.160	0.002	0.013
465	7.7334	0.162	0.160	0.002	0.012
466	7.7500	0.160	0.160	0.000	−0.001
467	7.7667	0.160	0.160	0.000	−0.002
468	7.7834	0.159	0.160	−0.001	−0.007
469	7.8000	0.159	0.160	−0.001	−0.007
470	7.8167	0.158	0.160	−0.002	−0.013
471	7.8334	0.158	0.160	−0.002	−0.012
472	7.8500	0.158	0.160	−0.002	−0.010
473	7.8667	0.159	0.160	−0.001	−0.003

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
474	7.8834	0.159	0.159	0.000	−0.003
475	7.9000	0.159	0.159	0.000	−0.001
476	7.9167	0.158	0.159	−0.001	−0.005
477	7.9334	0.158	0.159	−0.001	−0.004
478	7.9500	0.160	0.159	0.001	0.009
479	7.9667	0.160	0.159	0.001	0.008
480	7.9834	0.160	0.159	0.001	0.007
481	8.0000	0.160	0.159	0.001	0.006
482	8.0167	0.160	0.159	0.001	0.005
483	8.0334	0.160	0.159	0.001	0.004
484	8.0500	0.160	0.159	0.001	0.003
485	8.0667	0.160	0.160	0.000	0.003
486	8.0834	0.160	0.160	0.000	0.002
487	8.1000	0.160	0.160	0.000	0.001
488	8.1167	0.159	0.160	−0.001	−0.006
489	8.1334	0.159	0.160	−0.001	−0.005
490	8.1500	0.160	0.160	0.000	0.001
491	8.1667	0.160	0.160	0.000	0.001
492	8.1834	0.160	0.160	0.000	0.001
493	8.2000	0.159	0.160	−0.001	−0.005
494	8.2167	0.158	0.160	−0.002	−0.010
495	8.2334	0.158	0.159	−0.001	−0.009
496	8.2500	0.159	0.159	0.000	−0.002
497	8.2667	0.160	0.159	0.001	0.005
498	8.2834	0.160	0.159	0.001	0.005
499	8.3000	0.159	0.159	0.000	−0.002
500	8.3167	0.158	0.159	−0.001	−0.007
501	8.3334	0.159	0.159	0.000	−0.001
502	8.3500	0.160	0.159	0.001	0.006
503	8.3667	0.159	0.159	0.000	0.000
504	8.3834	0.160	0.159	0.001	0.006
505	8.4000	0.162	0.159	0.003	0.016
506	8.4167	0.160	0.160	0.000	0.002
507	8.4334	0.160	0.160	0.000	0.002
508	8.4500	0.160	0.160	0.000	0.002
509	8.4667	0.160	0.160	0.000	0.002
510	8.4834	0.160	0.160	0.000	0.001
511	8.5000	0.160	0.160	0.000	0.000
512	8.5167	0.160	0.160	0.000	−0.001
513	8.5334	0.160	0.160	0.000	−0.001

Sample Number	Time (min)	Measured Conc. (ppm)	Smoothed Conc. (ppm)	Absolute Error (dimen.)	Relative Error (dimen.)
514	8.5500	0.160	0.160	0.000	−0.001
515	8.5667	0.160	0.160	0.000	−0.001
516	8.5834	0.160	0.160	0.000	0.000
517	8.6000	0.160	0.160	0.000	0.000
518	8.6167	0.160	0.160	0.000	0.000
519	8.6334	0.160	0.160	0.000	0.000
520	8.6500	0.162	0.160	0.002	0.011
521	8.6667	0.162	0.160	0.002	0.010
522	8.6834	0.162	0.161	0.001	0.009
523	8.7000	0.162	0.161	0.001	0.008
524	8.7167	0.162	0.161	0.001	0.007
525	8.7334	0.162	0.161	0.001	0.006
526	8.7500	0.160	0.161	−0.001	−0.007
527	8.7667	0.160	0.161	−0.001	−0.007
528	8.7834	0.160	0.161	−0.001	−0.007
529	8.8000	0.162	0.161	0.001	0.004
530	8.8167	0.163	0.162	0.001	0.009

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