StreamVOC—A Deterministic Source-Apportionment Model to Estimate Volatile Organic Compound Concentrations in Rivers and Streams

Scientific Investigations Report 2006–5110

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By William Asher, David A. Bender, John S. Zogorski, and Roy C. Bartholomay

Scientific Investigations Report 2006–5110

U.S. Department of the Interior
DIRK KEMPTHORNE, Secretary

U.S. Geological Survey
P. Patrick Leahy, Acting Director

U.S. Geological Survey, Reston, Virginia: 2006

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Symbols, Derivatives, Units of Measurement, and Abbreviations

Symbol	Description	Unit of measurement
A_i	compound-dependent constant in T_w-dependent equation for H_i	
a	exposed stream surface seen by flow Q (note: $a = Q/h$)	m^2/s
B_i	compound-dependent constant in T_w-dependent equation for H_i	
$c_{d,i}$	concentration of contaminant i in stream immediately downstream from a hydraulic structure	mol/m^3
$c_{gw,i}$	concentration of contaminant i in ground water entering the stream	mol/m^3
c_i	overall concentration of contaminant i at point (x,y,z,t)	mol/m^3
Δc_i	concentration difference used to express the air-water mass transfer rate	mol/m^3
$c_{i,j}$	portion of the concentration of c_i that is due to source j	mol/m^3
c_0	concentration of contaminant i at the upstream end of the modeled region	mol/m^3
$c_{i,k}^{mod}$	surface-water concentration of contaminant i in zone k calculated by StreamVOC	mol/m^3
$c_{i,k}^{ss}$	surface-water concentration of contaminant i in zone k measured during the synoptic study	mol/m^3
$c_{s,i}$	water concentration of i that would be in "saturation" equilibrium at T_w	mol/m^3
$c_{u,i}$	concentration of contaminant i in stream immediately upstream from a hydraulic structure	mol/m^3
D_i	diffusivity of contaminant i in water at T_w	
D_{O2}	diffusivity of oxygen in water at 293.16 K	
d	depth of flow through hyporheic zone under a hydraulic structure	m
E_{20}	transfer efficiency for oxygen at 293.16 K at a hydraulic structure	
E_i	transfer efficiency of a contaminant with diffusivity equal to D_i at T_w but the solubility of oxygen at 293.16 K	
$E_i(H_i)$	transfer efficiency of a contaminant with diffusivity equal to D_i at T_w and solubility equal to H_i at T_w	
$\mathbf{F}$	Froude number of flow over a hydraulic structure	
$F_{air,i}$	the net air-water flux of VOC i	$mol/(m^2\text{-}s)$
F_{over}	fraction of total streamflow that flows over a dam or weir	
F_{under}	fraction of total streamflow that flows under dam or weir in hyporheic region	
f	compound and temperature specific correction factor for E_{20}	
f_i	local fraction for i of the total ambient atmospheric pressure	ppbv
g	acceleration of gravity	m^2/s
H	hydraulic head	m
H_i	compound- and temperature-dependent Henry's Gas Law constant for i	$m^3\text{-atm/mol}$
h	average stream depth at point $(x, y = 0, t)$	m
h_T	depth of tailwater downstream from weir	m
i	index for the contaminant of interest	
i,j	fractional change in concentration of i in source j	

Symbol	Description	Unit of measurement
$J_{\text{abs},i}$	the flux of VOC i from the atmosphere into the water	mol/(m^2-s)
$J_{\text{vol},i}$	the flux of VOC i from the water into the atmosphere	mol/(m^2-s)
j	index for the source of interest (note: maximum value of j is N_s)	
k	index for the point source of interest (note: maximum value of k is N_{ps})	
$k_{\text{deg},i}$	first-order degradation rate constant for i	1/s
$k_{\text{G},i}$	local mass transfer velocity for i through the air-side layer	m/s
$k_{\text{L},i}$	local mass transfer velocity for i through the water-side layer	m/s
$k_{\text{OA},i}$	local overall gas exchange velocity for VOC i	m/s
$k_{\text{OL},i}$	local overall air-water mass transfer velocity for i	m/s
k_2^{20}	rate constant for air-water mass transfer ("reaeration") of oxygen at 20°C ($T_w = 293.15$ K)	1/day
k^θ	rate constant for air-water mass transfer of oxygen at θ°C ($T_w = \theta + 293.15$ K)	1/day
L^2	total length of stream	km
$M_{i,j}$	mass of VOC i due to source j per unit volume of stream water	mol/s
M_i	mass of VOC i per unit volume of stream water	mol/s
MW$_i$	molecular weight of i	g/mol
$m_{\text{in},i}$	differential input rate for i from all local sources (including ground-water inflow)	mol/m-s
N	number of significant digits required in the model output	
$N_{\text{C},i}$	number of non-zero surface-water concentration measurements for i	
N_{ps}	number of point sources in system	
N_s	total number of sources in the system	
P	local total ambient atmospheric pressure	atm
p_i	local gas-phase pressure of i in the ambient air	atm
Q	streamflow at point (x, t)	m^3/s; ft^3/min
Q_{under}	streamflow under a hydraulic structure through the hyporheic zone	m^3/s
ΔQ	change in streamflow	ft^3/min
q	specific flow over a hydraulic structure ($= Q$ divided by structure width)	m^2/s
R	universal gas constant	m^3-atm/K-mol
R	Reynolds number of flow over hydraulic structure	
r	gas concentration deficit over a hydraulic structure	
r_{Hi}	gas concentration deficit for contaminant i	
S	cross-sectional area for flow through hyporheic zone under a hydraulic structure	m^2
s	submergence depth of sill lip for gated spillway	m
T_{A}	air temperature	°C
T_{w}	local bulk water temperature in the stream	K; °C
t	time	s
t_k	time the k'th point source enters the stream	s
U	wind speed	m/s
u	linear flow velocity in stream	m/s

Symbol	Description	Unit of measurement
$\overline{u}_{sz}$	average stream velocity over a subzone	m/s
$\Delta[VOC]_i$	difference between the modified source concentration and the source concentration determined from the synoptic study data set	
$[VOC]_{i,AVG}$	average concentration of the VOC over the synoptic study zone.	
$\overline{V}_i$	molar volume of i	cm^3/mol
w	average stream width at point (x, t)	m
x	longitudinal distance (Eulerian) along a stream ($x = 0$ at the *upstream* end of the modeled stream section)	m
Δx_{ps}	length of stream over which point source is active	m
Δx_{sz}	length of the subzone	m
y	horizontal transverse distance (Eulerian) in stream ($y = 0$ at stream center)	m
z	vertical transverse distance (Eulerian) in stream ($z = 0$ at stream surface)	m
$\alpha_{i,j}$	fraction of the concentration of c_i that is due to source j	
$\alpha_{d,i,j}$	fraction of concentration of c_i that is due to source j contaminant immediately downstream from a hydraulic structure	mol/m^3
α_{PS}	SA fraction from a point source	
α_{NPS}	SA fraction from a nonpoint source	
$\alpha_{u,i,j}$	fraction of concentration of c_i that is due to source j contaminant immediately upstream from a hydraulic structure	mol/m^3
$\alpha_{d,i,air}$	SA fraction for atmospheric source downstream from the hydraulic structure	mol/m^3
$\alpha_{u,i,air}$	upstream SA fraction for the atmospheric source term i	mol/m^3
β_i	normalized fractional change of the concentration of VOC$_i$ in source j	
$\gamma_{i,j}$	normalized difference between measured and modeled concentrations	
δ	Kroenecker delta function	
η	head loss across hydraulic structure	m
θ	bulk stream-water temperature (note: $\theta = T_w - 273.15$)	°C
κ	hydraulic conductivity	m/s
ν	kinematic viscosity of water	m^2/s
$\phi_{gw}(t)$	rate at which ground water enters or leaves the stream water as a function of time	m^3/s^2
ϕ_{ps}	flow of water entering stream from a point source	m^3/s
Φ_{gw}	rate at which streamflow discharge is lost by water outflow to ground water or a point withdrawal	m^3/s^2
$\Phi_{gw}c_i$	differential rate at which discharge of i is reduced due to water outflow to ground water	mol/s^2
Φ_{out}	differential rate at which stream-water discharge is lost by water outflow to ground water or to a point withdrawal	m^3/s^2
$\rho_{i,j}$	fractional change in concentration of i in source j	
$\tau_{0.5,i}$	degradation half-life of i	
χ_i^2	reduced chi-square optimization parameter	m/s

Derivatives		
dc_i/dt	time rate of change of concentration of i at point (x,t)	mol/m^3-s
$d\alpha_{i,j}/dt$	time rate of change in source apportionment of source j for VOC$_i$	
$dM_{i,j}/dt$	change in mass of VOC i due to source j in the time interval defined by dt	mol/s^2
dM_i/dt	total change in mass of VOC i in the time interval defined by dt	mol/s^2
dQ/dt	change in streamflow volume in the time interval defined by dt	m^3/s^2

Units of measurement	
atm	atmosphere
cm^3/mol	cubic centimeters per mole
ft	feet
°C	degrees Celsius
ft^3/min-km	cubic foot per minute per kilometer
g/mol	grams per mole
K	degrees Kelvin
km	kilometer
m	meter
m/s	meters per second
m^2/s	meters squared per second
m^3/s	cubic meters per second
m^3-atm/K-mol	cubic meters atmosphere per Kelvin per mole
m^3/s-km	cubic meters per second per kilometer
m^3/s^2	cubic meters per square second
m^3-atm/mol	cubic meters atmosphere per mole
mol	moles
mol/m-s	moles per meter per second
mol/s^2	moles per square second
mol/m^3	moles per cubic meter
mol/m^3-s	moles per cubic meter per second
ppbv	parts per billion by volume
s	second
μg/L	micrograms per liter
μg/L-s	micrograms per liter per second

Abbreviations	
ACE	acetone
BEN	benzene
CLF	chloroform
1-D	one-dimensional
1,1-DCA	1,1-dichloroethane
cis-1,2-DCE	*cis*-1,2-dichloroethene
DEQ	differential equation
EDT	Eastern Daylight Time
GPS	global positioning system
MDL	method detection limit

Abbreviations—Continued	
MTBE	methyl *tert*-butyl ether
NAWQA	National Water-Quality Assessment Program of the U.S. Geological Survey
ND	not detected
NPS	nonpoint source
PS	point source
PCE	perchloroethene (also known as tetrachloroethene)
SA	source apportionment
TCE	trichloroethene
VOC	volatile organic compound
<	less than
>	greater than

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By William E. Asher, David A. Bender, John S. Zogorski, and Roy C. Bartholomay

Abstract

This report documents the construction and verification of the model, StreamVOC, that estimates (1) the time- and position-dependent concentrations of volatile organic compounds (VOCs) in rivers and streams as well as (2) the source apportionment (SA) of those concentrations. The model considers how different types of sources and loss processes can act together to yield a given observed VOC concentration. Reasons for interest in the relative and absolute contributions of different sources to contaminant concentrations include the need to apportion: (1) the origins for an observed contamination, and (2) the associated human and ecosystem risks. For VOCs, sources of interest include the atmosphere (by absorption), as well as point and nonpoint inflows of VOC-containing water. Loss processes of interest include volatilization to the atmosphere, degradation, and outflows of VOC-containing water from the stream to local ground water.

This report presents the details of StreamVOC and compares model output with measured concentrations for eight VOCs found in the Aberjona River at Winchester, Massachusetts. Input data for the model were obtained during a synoptic study of the stream system conducted July 11–13, 2001, as part of the National Water-Quality Assessment (NAWQA) Program of the U.S. Geological Survey. The input data included a variety of basic stream characteristics (for example, flows, temperature, and VOC concentrations). The StreamVOC concentration results agreed moderately well with the measured concentration data for several VOCs and provided compound-dependent SA estimates as a function of longitudinal distance down the river. For many VOCs, the quality of the agreement between the model-simulated and measured concentrations could be improved by simple adjustments of the model input parameters. In general, this study illustrated: (1) the considerable difficulty of quantifying correctly the locations and magnitudes of ground-water-related sources of contamination in streams; and (2) that model-based estimates of stream VOC concentrations are likely to be most accurate when the major sources are point sources or tributaries where the spatial extent and magnitude of the sources are tightly constrained and easily determined.

Introduction

The National Water-Quality Assessment (NAWQA) Program of the U.S. Geological Survey seeks to understand the sources and processes that determine the concentrations, transport, and fate of contaminants in the natural waters of the United States (Gilliom and others, 1995). Contaminant groups of interest include volatile organic compounds (VOCs), pesticides, nutrients, trace elements, and major ions. For urban streams, NAWQA results indicate the frequent presence of multiple dissolved VOCs (Gilliom and others, 1995; Lopes and Price, 1997). An adequate understanding, however, does not exist for the identities and relative roles of the typical contaminant sources that lead to the observed VOC concentrations, nor for the coupled manners in which physical, chemical, and biological processes in streams act on those contributions to yield observed position- and time-dependent concentrations. There is interest in the continued development of "source apportionment" (SA) modeling principles for use in tracking how multiple VOC sources and sinks can combine to yield a given observed concentration at some stream point (x,y,z,t). Reasons for interest in the relative and absolute contributions of different sources to VOC concentrations include the need to apportion: (1) the origins for observed contamination; and (2) the associated human and ecosystem risks.

Pankow and others (2006) provided a theoretical framework for SA modeling in streams. For each contaminant i and each stream point (x,y,z,t), they define $\alpha_{i,1}, \alpha_{i,2}\ldots\alpha_{i,Ns}$ as the SA fractions due to the total number of different sources (N_s) acting along a stream, which can be written as:

$$\alpha_{i,j} = \frac{c_{i,j}}{c_i} = \frac{M_{i,j}}{M_i}, \qquad (1)$$

where $c_{i,j}$ (mol/m^3) is the portion of the concentration of c_i (mol/m^3) that is due to source j. For each i, $\alpha_{i,1} + \alpha_{i,2} + \ldots + \alpha_{i,Ns} = 1$, M_i (mol/s) is the rate at which the stream discharges compound i, and $M_{i,j}$ (mol/s) is the j-related portion of that discharge.

When a contaminant i is subject to air/water partitioning according to Henry's Gas Law, as are the VOCs, then $c_{s,i}$ is

defined as the water concentration of i that would be present at equilibrium with the local air. Pankow and others (2006) described three possibilities: (1) $c_i > c_{s,i}$ so that i is volatizing from the stream to the atmosphere; (2) $c_i < c_s$, so that i is being absorbed from the atmosphere into the stream; or (3) $c_i = c_{s,i}$ so that i is neither volatilizing from the stream, nor being absorbed from the atmosphere. The direction and magnitude of the flux will thus depend on the local values of the concentrations in the adjacent air and water phases, and on H_i (m^3-atm/mol), which is the compound- and temperature-dependent Henry's Gas Law equilibrium constant.

Pankow and others (2006) showed that the first two possibilities described previously ($c_i > c_{s,i}$ and $c_i < c_{s,i}$) lead directly to two SA rules governing calculation of α values for VOCs:

1. wherever and whenever a stream is absorbing i from the atmosphere, the air-to-water flux causes a corresponding increase in the particular $c_{i,j}$ that is related to the atmosphere; and

2. wherever and whenever volatilization loss occurs from the stream, the water-to-air loss acts to diminish all of the local $c_{i,j}$ (including the particular, atmospheric $c_{i,j}$) by degrees that are in proportion to their corresponding local $\alpha_{i,j}$ values.

Pankow and others (2006) explained that the second rule extends to losses by mechanisms other than volatilization (for example, it extends to losses of i from the stream due to biological and abiotic degradation, water removal by infiltration to ground water, and others). As a result, at any point (x,y,z,t), the set of $\alpha_{i,j}$ values for a given contaminant i will not change whenever contaminant mass is lost from a stream; changes in a set of $\alpha_{i,j}$ only can occur when one or more sources act to add contaminant mass at (x,y,z,t) (Pankow and others, 2006).

A deterministic SA model, StreamVOC, was developed to estimate VOC concentrations in rivers and streams. The model considers how different types of sources and loss processes can act together to yield an observed VOC concentration.

Purpose and Scope

The purpose of this report is to document StreamVOC, which is a source-apportionment model to estimate total VOC concentrations and the SA fractions as a function of distance in rivers and streams. User instructions and information needs for running StreamVOC are described. The numerical performance and behavior of the model is verified using input data constructed for a hypothetical stream and input data collected during a source-synoptic study of the Aberjona River in Winchester, Massachusetts. As basic input, StreamVOC requires the river depth and width as a function of position, river flow rates, inflows from tributaries, ground-water inflow and loss along the river, and VOC concentrations in tributaries and ground-water sources. For StreamVOC, the river is assumed to be well mixed vertically and accounts for VOC losses through biological/chemical degradation, ground-water recharge, and air-water gas exchange. User-entered model parameters include

wind speed, air and water temperature, atmospheric pressure, relative humidity, atmospheric VOC concentration, stream depth as a function of position, stream width as a function of position, VOC inputs to the stream other than the atmosphere, surface-water degradation rates, diffusivity parameters, solubility parameters, and the molecular weight of the VOC.

Acknowledgments

Description and Theoretical Basis of StreamVOC

This section presents a general description, governing equations, and physicochemical parameterizations for StreamVOC. Model operation and numerical methods are described.

General Description

The one-dimensional (1-D) version of StreamVOC described in this report assumes that a stream with total length L (km) can be divided into a finite number of separate, longitudinal zones. It is assumed that each zone can be characterized by a constant average stream depth h (m) and a constant average width w (m). Within a given zone, however, the total streamflow Q (m^3/s) and velocity u (m/s) may change due to streamflow gains (or losses) from (to) ground water. The zone boundaries are defined as the particular distances x along the stream at which there is: (1) a change in h or w; (2) a tributary inflow that may or may not contain contaminant(s) of interest; and/or (3) one or more point sources that add contaminant mass. Because of the third possibility, a set of model zones, in general, will not correspond to a set of stream "reaches" that would be defined by flow characteristics alone. Within a given zone, contaminant mass may enter a stream from a distributed source (as from the nonpoint inflow of contaminated ground water), a point source (such as from tributary inflow), or from the atmosphere. Contaminant mass may be lost within a zone by volatilization to the atmosphere, degradation, and/or outflow of stream water to local ground water.

Figure 1 shows a hypothetical stream with four zones each characterized by a depth (h_i) and width (w_i) and four VOC sources (the atmosphere, two point sources, and a distributed source related to ground-water inflow). There also are two areas of stream outflow to ground water. The stream data required to initialize the model presented are h_i, w_i, and Q_i for each zone, the atmospheric VOC concentration, the VOC concentrations in
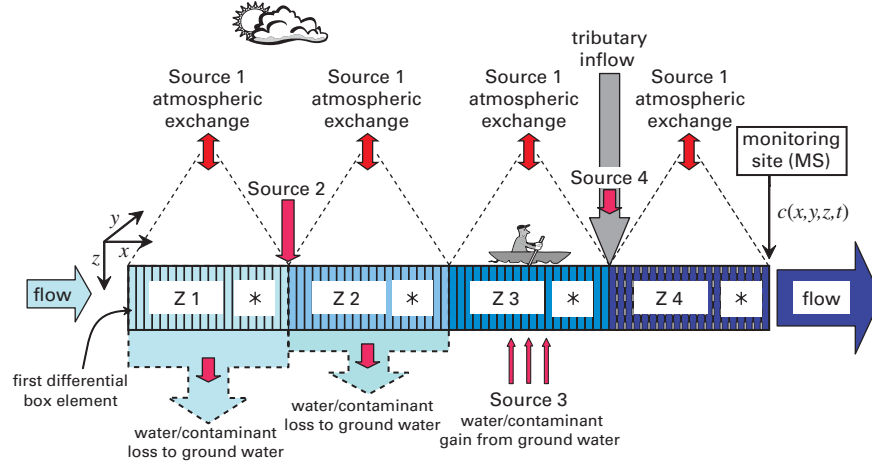
Figure 1. Schematic representation of a portion of an example stream that is characterized by a series of four distinct hydrologic zones (Z1–Z4). The zone boundaries correspond to changes in stream width or depth, or could reflect the presence of tributaries or point sources. Monitoring site (MS) is shown at which the concentration c(x,y,z,t) is of particular interest. For modeling purposes, each zone is discretizied into a series of sequential box elements. Four sources (S1–S4) of a volatile organic compound (VOC) of interest are shown. The possibility of contaminant loss by degradation within *each* box element in each reach is represented with the symbol ∗. The VOC will tend to exchange with the atmosphere from the surface area of each box element. On the ground-water side, water loss and associated VOC loss, or water gain and associated VOC gain, may be prescribed for each differential box element.

each point source and in ground-water inflow, the ground-water inflow and outflow volumes, and the flow volumes for the two point sources. Other ancillary data required include the air/water temperature, atmospheric pressure, average wind speed, and knowledge of the molecular diffusivity and solubility of the VOC.

Parameters are entered through an ASCII parameter file. Numerical output from the model is displayed graphically and saved to an optional ASCII data file.

Governing Equations

StreamVOC tracks the SA of a VOC in a Lagrangian manner as a parcel of water moves downstream. At any given point in the stream, the volume of the parcel corresponds to 1 second's worth of flow, and therefore equals $Q \times 1$ s. Consequently, the flow gains and losses experienced by the stream cause the parcel to undergo changes in volume as a function of t. Changes in c_i can thus be caused by contaminant addition or loss, as well as by changes in Q. (This approach simplifies consideration of the effects of dilution and mixing at confluences because flows at confluences are directly additive.) For VOC i, the time rate of change in a vertically and laterally mixed stream thus can be written as:

$$\frac{dc_i}{dt}(\text{mol/m}^3\text{-s}) = \frac{(aF_{\text{air},i} + m_{\text{in},i}u - \Phi_{\text{out}}c_i)}{Q} -$$

$$k_{\text{deg},i}c_i - \frac{c_i}{Q}\frac{dQ}{dt} , \qquad (2)$$

where $a = wu$ (m^2/s) is the stream surface area in contact with atmosphere corresponding to 1 second's worth of flow; $F_{\text{air},i}$ (mol/m^2-s) is the net air-water VOC flux and may be positive or negative if the stream is under- or supersaturated, respectively, with respect to the local atmospheric VOC concentration; $m_{\text{in},i}$ (mol/m-s) is differential input rate for i given as the mass inflow in terms of moles per unit time per distance along the river from local point sources, or from ground-water inflow (but not from the atmosphere, which is considered separately by the term $aF_{\text{air},i}$); Φ_{out} (m^3/s^2) is differential rate at which stream-water discharge is lost by water outflow to ground water or to a point withdrawal (Φ_{out} is "positive-definite": it can be positive or zero, but cannot be negative); and $k_{\text{deg},i}$ (1/s) is first-order degradation rate constant for i. The term (c_i/Q)(dQ/dt) accounts for changes in c_i due to changes in Q alone.

As described in Pankow and others (2006), there are two complementary approaches for calculating $F_{\text{air},i}$. In the first method, $F_{\text{air},i}$ is calculated as a net flux using the relation

$$F_{\text{air},i} = k_{\text{OL},i}(c_{\text{s},i} - c_i) , \qquad (3)$$

where $k_{\text{OL},i}$ (m/s) is the local air-water mass transfer velocity of i, and $c_{\text{s},i}$ is the saturation concentration of the volatile species with respect to Henry's Gas Law. Using the net flux approach, the atmosphere is a source of VOC only when the concentration difference, ($c_{\text{s},i} - c_i$), is positive; when the concentration difference is zero or negative, the atmosphere is not a source of VOC.

The second method is called the component flux method and, in this case $F_{\text{air},i}$, is calculated as the difference between the

absorptive flux into the stream, J_{abs}, and the volatilization from the stream, J_{vol}. The absorptive flux is calculated as

$$J_{abs} = k_{OL,i} c_{s,i} \ , \tag{4}$$

and J_{vol} is given by

$$J_{vol} = k_{OL,i} c_i \ , \tag{5}$$

so that as long as the partial pressure of the VOC in the atmosphere is not equal to zero, the air is a source of VOC to the stream.

The change in Q with time, dQ/dt, is calculated internally by StreamVOC based on position-dependent user inputs for h, w, u, Φ_{out}, and the source flows. Conceptually, dQ/dt is given by

$$\frac{dQ}{dt} = \phi_{gw}(t) + \sum_{k=1}^{N_s} \phi_{ps,k} \delta(t - t_k) \ , \tag{6}$$

where $\phi_{gw}(t)$ (m³/s) is the ground-water inflow or loss rate to the stream as a function of time, $\phi_{ps,k}$ (m³/s) is the flow volume added by the k'th point source (or removed by the k'th point withdrawal), and $\delta(t - t_k)$ is the Kroenecker delta function for time t_k, or the time that the k'th point source enters the stream. In the case where $\phi_{gw}(t)$ is positive (that is, ground-water inflow to the stream) the VOC mass inflow to the stream due to the ground water, $m_{in,i}(GW)$ is defined as

$$m_{in,i}(GW) = \frac{\phi_{gw}(t) c_{gw,i}(t)}{u} \ , \tag{7}$$

where $c_{gw,i}(t)$ is the ground-water concentration of i at time t. In the case where $\phi_{gw}(t)$ is negative, $\Phi_{out} = -\phi_{gw}(t)$. For $\phi_{ps,k}$, the point-source VOC mass inflow to the stream, $m_{in,i}(PS)$, is equal to

$$m_{in,i}(PS) = \frac{\phi_{ps,k} c_{ps,i,k} \delta(t - t_k)}{u} \ , \tag{8}$$

where $c_{ps,i,k}$ is the concentration of i in point source k. In the case where $\phi_{ps,k}$ is a point withdrawal, $\Phi_{out} = \phi_{ps,k}$.

The source apportionment fractions for the j sources (where j equals the sum of the number of discrete ground-water sources and the k point sources) are readily calculated from the equations for c_i, M_i, and Q given previously (equations 1 and 2). Differentiation of equation 1 yields

$$\frac{d\alpha_{i,j}}{dt} = \frac{1}{M_i} \left(\frac{dM_{i,j}}{dt} - \alpha_{i,j} \frac{dM_i}{dt} \right) , \tag{9}$$

where the units of both $dM_{i,j}/dt$ and dM_i/dt are mol/s². During execution, only the atmosphere and one additional source j at a time is considered in the model. The functional form depends slightly on whether the net flux or component flux method is being used. For the net flux method and the atmosphere being a source of a VOC to the stream (for example, invasion, $F_{air,i} > 0$), $dM_{i,j}/dt$ for source j is calculated by

$$\frac{dM_{i,j}}{dt} = m_{in,i} \, u - \alpha_{i,j} (\Phi_{gw} c_{gw,i} + k_{deg,i} \, c_i Q) \ , \tag{10}$$

and when the atmosphere is a sink of VOC (for example, evasion, $F_{air,i} < 0$), $dM_{i,j}/dt$ is calculated by

$$\frac{dM_{i,j}}{dt} = m_{in,i} \, u - \alpha_{i,j} (\Phi_{gw} c_{gw,i} + k_{deg,i} c_i Q - a F_{air,i}) \ . \tag{11}$$

Most importantly, if $F_{air,i} > 0$ and the atmosphere is a source of a VOC, $dM_{i,air}/dt$ is calculated by

$$\frac{dM_{i,air}}{dt} = a F_{air,i} - \alpha_{i,air} (\Phi_{gw} c_{gw,i} + k_{deg,i} c_i Q) \ , \tag{12}$$

whereas the source fraction for the atmospheric source remains unchanged if the river is losing the VOC to the atmosphere so that $F_{air,i} \leq 0$.

In the case of source apportionment calculations using the component flux method, no distinction needs to be made between invasion and evasion, and equations 10 and 11 reduce to

$$\frac{dM_{i,j}}{dt} = m_{in,i} \, u - \alpha_{i,j} (\Phi_{gw} c_{gw,i} + k_{deg,i} c_i Q - a J_{vol,i}) \tag{13}$$

for nonatmospheric sources, and the atmospheric source in equation 12 becomes

$$\frac{dM_{i,air}}{dt} = a J_{abs,i} - \alpha_{i,air} (\Phi_{gw} c_{gw,i} + k_{deg,i} c_i Q + a J_{vol,i}) \tag{14}$$

for the atmospheric source. Comparing equations 10 and 11 for the net flux approach with equation 13 for the component flux method and comparing equation 12 (net flux method) with equation 14 (component flux method) shows that when the concentration of VOC in the atmosphere is equal to zero (that is, $c_s = 0$) the two ways of treating the atmospheric source are mathematically identical.

The final relation necessary for application of equation 9 is a relation for dM_i/dt. Because $c_i = M_i/Q$, it can be shown based on equation 2 that

$$\frac{dM_i}{dt} = a F_{air,i} + m_{in,i} u - \Phi_{gw} c_{gw,i} - k_{deg,i} c_i Q \ , \tag{15}$$

which can be substituted into equation 9 along with the applicable form for $dM_{i,j}/dt$ to allow calculation of $d\alpha_{i,j}/dt$.

Comparison of the different formulations of the air-water gas flux shows that the main difference between the two methods is in the behavior of the SA. For example, in the net flux method, when $c_i = c_{s,i}$, the system is in equilibrium, and there is no change in the SA. Similarly, when $c_i > c_{s,i}$, the stream is losing the VOC to the atmosphere, and again there is no change in the SA. In contrast, in the component flux method, whenever $c_{s,i} > 0$, the atmosphere is a source of the VOC to the stream, and in the absence of other sources $\alpha_{i,air}$ will increase. However, it is important to understand that as far as the change in the total concentration c_i is concerned, both the net flux method and the component flux method are identical.

Theoretical estimates of air-water gas fluxes at waterfalls (McLachlan and others, 1990) and the results of recent tracer studies (Caplow and others, 2004) have shown that waterfalls and weirs can be dominant mechanisms for air-water exchange

in river systems. As described by Gulliver and others (1998), gas exchange at a hydraulic structure in a stream is given in terms of the transfer efficiency, E_i, defined as

$$E_i = \frac{(c_{d,i} - c_{u,i})}{(c_{s,i} - c_{u,i})} , \qquad (16)$$

where $c_{u,i}$ is the concentration of the species upstream from the structure, and $c_{d,i}$ is the concentration downstream from the structure. E_i is a function of the physical characteristics of the hydraulic structure, the molecular diffusivity of i, and the solubility of i.

Regardless of the functional form used for E_i, air-water exchange of i at a hydraulic structure in a stream is treated as a step function change in its concentration. The effect this has on the SA is determined by whether the net flux or component fluxes approach is being used.

For the net flux method, in the case where the net flux of i is from the water to the air (for example, evasion), $c_{d,i} < c_{u,i}$ as defined by equation 16. In this case, there will be no change in the SAs because all sources were assumed to have lost a proportional fraction based on the assumption that volatilization acts to decrease all of the local $c_{i,j}$ in proportion to their local $\alpha_{i,j}$ values (see SA rule 2 given previously in the Introduction section). In the case of net flux of i from the air to the water (for example, invasion), $c_{d,i} > c_{u,i}$. In contrast to evasion, the change in SA for invasion of i must be calculated because mass of i was added to the atmospheric source fraction. Assuming that Q is constant upstream and downstream from the structure, the source fractions for the nonatmospheric sources immediately downstream from the hydraulic structure are

$$\alpha_{d,i,j} = \frac{\alpha_{u,i,j} c_{u,i}}{c_{d,i}} , \qquad (17)$$

where $\alpha_{d,i,j}$ is the SA fraction for source j immediately downstream from the structure, and $\alpha_{u,i,j}$ is the SA fraction for source j immediately upstream from the structure. The SA fraction for the atmospheric source downstream from the structure, $\alpha_{d,i,air}$, can be written as

$$\alpha_{d,i,air} = \frac{(c_{d,i} - c_{u,i}) + \alpha_{u,i,air} c_{u,i}}{c_{d,i}} , \qquad (18)$$

where $\alpha_{u,i,air}$ is the upstream SA fraction for the atmospheric source term of i.

When the component flux method is being used to estimate $\alpha_{i,j}$, SAs must be calculated after aeration by the hydraulic structure for both evasion and invasion. In this case, it is more convenient to define the effect on the SAs in terms of E_i. The SA downstream from the hydraulic structure of the nonatmospheric sources is defined as

$$\alpha_{d,i,j} = \alpha_{u,i,j} \left[\frac{c_{u,i}(1 - E_i)}{c_{d,i}} \right] , \qquad (19)$$

which applies for both invasion and evasion. Similarly, $\alpha_{d,i,air}$ is equal to

$$\alpha_{d,i,air} = \frac{\alpha_{u,i,air} c_{u,i}(1 - E_i) + E_i c_{s,i}}{c_{d,i}} , \qquad (20)$$

which applies to both invasion and evasion.

Substantial flow of water under the hydraulic structure is possible, which will decrease the apparent aeration efficiency of the structure and change the relations given previously for SA. Darcy's Law relates the flow under a structure to the hydraulic conductivity and hydraulic head as

$$Q_{under} = \frac{\kappa S H}{d} , \qquad (21)$$

where Q_{under} (m³/s) is the flow underneath the hydraulic structure, κ (m/s) is hydraulic conductivity, S (m²) is cross-sectional area for flow under the structure, H (m) is total hydraulic head or pressure gradient, and d (m) is depth of flow under the structure. The effect of Q_{under} on aeration can be viewed in terms of dilution, where the flow over the structure (for example, $Q - Q_{under}$) has its VOC concentration changed as specified by equation 16 and the flow under the structure has no change in VOC concentration. These two waters are assumed to mix completely downstream from the structure so that c_i immediately downstream from the structure can be written as

$$c_i = \frac{c_{u,i} Q_{under} + c_{d,i}(Q - Q_{under})}{Q} , \qquad (22)$$

where $c_{d,i}$ is the VOC concentration in the water that flowed over the weir as calculated using equation 16.

The effect of this flow on SA can be expressed in terms of the fraction of the total flow going over the structure, F_{over}, which is defined as

$$F_{over} = \frac{Q - Q_{under}}{Q} . \qquad (23)$$

The relations for the change in SA are as follows: equation 17 is unchanged when flow under the weir is taken into account; however, equations 18–20 become

$$\alpha_{d,i,air} = \frac{F_{over}(c_{d,i} - c_{u,i}) + \alpha_{u,i,air} c_{u,i}}{c_{d,i}} , \qquad (24)$$

$$\alpha_{d,i,j} = \alpha_{u,i,j} \left[\frac{c_{u,i}(1 - F_{over} E_i)}{c_{d,i}} \right], \qquad (25)$$

and

$$\alpha_{d,i,air} = \frac{\alpha_{u,i,air} c_{u,i}(1 - F_{over} E_i) + F_{over} E_i c_{s,i}}{c_{d,i}} , \qquad (26)$$

respectively.

Equations 2, 6, 9, and 15 comprise a set of coupled differential equations (DEQs) that can be solved by numerical integration based on data inputs for the stream characteristics by zone, and data inputs for the strengths and locations of the sources acting on the stream. In the following sections of the report, it will be assumed that all flows are steady, all sources and sinks are steady, and vertical/lateral mixing is complete at each point along the length of the stream. For each VOC i, these assumptions simplify the functionality of each $c_i(x,y,z,t)$ to $c_i(x)$, and simplify the functionalities of each $\alpha_{i,j}(x,y,z,t)$ to $\alpha_{i,j}(x)$.

Physicochemical Parameterizations

The air-water transfer velocity, $k_{OL,i}$, controls the kinetic rate of transfer of i across the air/water interface. Values of $k_{OL,i}$ were estimated using the "two-film model" (Liss and Slater, 1974) of air-water gas transfer in which it is postulated that $k_{OL,i}$ is determined by diffusion-limited molecular transfer through two thin, stagnant layers. One of those layers is on the water side, and the other is on the air side. According to that model,

$$\frac{1}{k_{OL,i}} = \frac{1}{k_{L,i}} + \frac{RT_w}{H_i k_{G,i}}, \qquad (27)$$

where $k_{L,i}$ (m/s) is the mass transfer velocity for i through the water-side layer, $k_{G,i}$ (m/s) is the mass transfer velocity for i through the air-side layer, R (m^3-atm/K-mol) is the universal gas constant, T_w (K) is the water temperature, and H_i (m^3-atm/mol) is the Henry's Gas Law constant for i at T_w.

StreamVOC estimates $k_{L,i}$ values based on estimated values of k_2^{20} (day^{-1}), which is the rate constant for air-water transfer of oxygen at 20°C ($T_w = 293.15$ K). For streams where the overall depth is greater than 0.274 m and less than 11.3 m and the flow velocity is greater than 0.058 m/s and less than 1.28 m/s, k_2^{20} can be estimated according to the following equation (O'Conner and Dobbins, 1958):

$$k_2^{20} = 3.93 \frac{u^{0.5}}{h^{1.5}}. \qquad (28)$$

In the case of streams with 0.274 m > h > 0.119 m and u > 0.04 m/s, the relation of Owens and others (1964) is used. It has the same functional form as equation 28, but the constant is 6.92 instead of 3.93, the exponent for u is 0.73 instead of 0.5, and the exponent for h is 1.75 instead of 1.5. For streams with u < 0.04 m/s and h > 0.119 m, gas transfer is assumed to be driven by wind stress, and $k_{L,i}$ is calculated using the wind speed relation of Wanninkhof and others (1991). This is

$$k_L = 1.25 \times 10^{-6} \sqrt{\frac{600 D_i}{\nu}} \, U^{1.64}, \qquad (29)$$

where k_L is given in m/s, ν is the kinematic viscosity of water in cm^2/s (for D_i in cm^2/s), and the wind speed, U, is in m/s. Although the Wanninkhof and others (1991) relation is defined in terms of U_{10}, which is the wind speed measured at a height of 10 m for neutral atmospheric stability, it is understood that values for U_{10} will not be available for most applications of StreamVOC. In these cases, measurements of wind speed made at heights other than 10 m can be used without substantial loss in accuracy of the model. StreamVOC prohibits using stream depths less than 0.119 m, regardless of u.

StreamVOC corrects k_2^{20} values to any temperature θ (°C) using the following equation (Rathbun, 2000):

$$k_2^{\theta} = k_2^{20}(1.0241)^{\theta - 20}, \qquad (30)$$

where θ is equal to T_w - 273.15. Values of $k_{L,i}$ are obtained by the following equation (Rathbun, 2000):

$$k_{L,i} = \frac{2.52 h(\bar{V}_i)^{-0.301} k_2^{\theta}}{86400}, \qquad (31)$$

where $\bar{V}_i$ (cm^3/mol) is the molar volume of i.

StreamVOC estimates $k_{G,i}$ values based on the rate constant for air-water transfer of water itself, the molecular weight MW_i (g/mol), the wind speed U (m/s), and T_A (°C) according to the following equation (Rathbun, 2000):

$$k_{G,i} = \frac{4.42 \, MW_i^{-0.462}(416 + 156 \, U)\exp[0.00934(T_A - 26.1)]}{86400}. \qquad (32)$$

The quantity that acts together with $k_{OL,i}$ to determine the air-water flux of i (see equation 2) is

$$\Delta c_i = c_{s,i} - c_i. \qquad (33)$$

As previously stated, $c_{s,i}$ is the water concentration of i that would be present at T_w under the condition of "saturation" equilibrium by Henry's Gas Law with the gas-phase pressure p_i (atm) in the local ambient air. This Henry's Gas Law saturation equilibrium concentration is determined from

$$c_{s,i} = \frac{p_i}{H_i}, \qquad (34)$$

where

$$p_i = f_i \frac{P}{10^9}, \qquad (35)$$

with f_i (parts per billion by volume, ppbv) equal to the i-related fraction of the local total ambient atmospheric pressure P (atm). Recently, for ambient urban air in the United States, Pankow and others (2003) determined that f_i < 10 ppbv for most contaminant VOCs of interest. (For nitrogen in the earth's atmosphere, $f_{N_2} = 0.78 \times 10^9$ ppbv.)

StreamVOC can accept user-supplied, T_w-dependent H_i values. It also can calculate H_i values based on T_w and either the polynomial relation of Wanninkhof (1992), or the following exponential expression (Reid and others, 1987; Rathbun, 2000):

$$H_i(T_w) = \exp\left[A_i - \frac{B_i}{T_w}\right], \qquad (36)$$

where A_i and B_i are compound dependent constants. An advantage of equation 36 is that A_i and B_i values are available for many compounds of environmental interest (Rathbun, 2000).

Relations for E_i, as defined in equation 16, are available for sharp-crested weirs, ogee-crested weirs, and gated spillways (Gulliver and others, 1998). In general, E_i is not known for particular VOCs and must be estimated from the transfer efficiency of oxygen measured at 293.16 K. In the case of a sharp-crested weir, the transfer efficiency of oxygen at 293.16 K, E_{20}, is given by Avery and Novak (1978) as

$$E_{20} = 1 - \left(\frac{1}{1 + 0.24 \times 10^{-4} F^{1.79} R^{0.53}}\right)^{1.115}, \qquad (37)$$

where $\mathbf{F}$ and $\mathbf{R}$ are the Froude and Reynolds numbers, respectively, of the flow over the hydraulic structure. $\mathbf{F}$ is expressed in terms of the specific flow of the stream over the weir as

$$\mathbf{F} = \left(\frac{8g\eta^3}{q^2}\right)^{1/4}, \tag{38}$$

where g (m/s^2) is the acceleration of gravity, η (m) is the head loss across the structure, and q (m^2/s) is the specific flow over the weir (defined as Q divided by the width of the weir). $\mathbf{R}$ is defined in terms of q as q/ν, where ν (m^2/s) is the kinematic viscosity of water at 293.16 K. In the case of an ogee-crested weir, E_{20} is given by Rindels and Gulliver (1991) as

$$E_{20} = 1 - \exp\left(\frac{-0.263\eta}{1 + 0.215q} - 0.203h_\mathrm{T}\right), \tag{39}$$

where h_T (m) is the depth of the weir tailwater. The transfer efficiency of a gated spillway (Wilhelms, 1988) is defined as

$$E_{20} = 1 - \exp\left(-0.0086\frac{\eta q}{s} - 0.118\right), \tag{40}$$

where s (m) is the submergence depth of the gate lip.

Following Urban and others (2001), E_{20} is converted to the equivalent transfer efficiency for the VOC i at the system water temperature T_w using:

$$E_i = 1 - (1 - E_{20})^f, \tag{41}$$

where E_i is the transfer efficiency of i, and f is a compound and temperature specific correction factor given by

$$f = \left(\frac{D_i}{D_{\mathrm{O2}}}\right)^{1/2}[1.0 + 0.02103(T_\mathrm{w} - 293.16) + \tag{42}$$

$$8.261 \times 10^{-5}(T_\mathrm{w} - 293.16)^2],$$

where D_{O2} is the molecular diffusivity of oxygen in water at 293.16 K, and D_i is the diffusivity of i in water at the water temperature T_w.

McLachlan and others (1990) have shown that the transfer efficiency of i at a waterfall also is a function of its solubility. Therefore, E_i calculated using equation 40 represents the efficiency of a hypothetical VOC with diffusivity equal to D_i but the solubility of oxygen at 293.16 K. If the solubility of i is very much different from that of oxygen, E_i must be corrected for the change in H_i based on the relations presented by McLachlan and others (1990). From those relations, it can be shown that for E_i corrected to account for changes in solubility, $E_i(H_i)$ is approximately equal to

$$E_i(H_i) = 1 - \frac{1}{r_{Hi}}, \tag{43}$$

where r_{Hi} is defined as:

$$r_{Hi} = \left(r + \frac{RT_\mathrm{w}}{150H_i}\right)\left(1 + \frac{RT_\mathrm{w}}{150H_i}\right)^{-1} \tag{44}$$

and r is the gas concentration deficit defined by $r = 1/(1 - E_i)$ (McLachlan and others, 1990).

Flow under any hydraulic structure through the hyporheic zone is parameterized as a "worst-case" estimate using a hydraulic conductivity of 0.01 m/s, which is the value typical of coarse gravel. For most reasonable values of S (cross-sectional area for flow through the hyporheic zone), H, and d (depth of flow through the hyporheic zone), this results in approximately 20 percent of the total flow going under the structure rather than over the top. Rather than add additional complexity to the model by explicitly calculating Q_under, it has been assumed that it will be $0.2Q$ for all structures in the stream. Therefore, the maximum expected effect of aeration by dams and weirs can be turned on and off by a simple flag in the model.

Model Operation and Numerical Methods

StreamVOC is written in Fortran 90 (Appendix 1) and uses a fourth-order Runge-Kutta integration subroutine (Hall and Watt, 1976) to solve the governing set of coupled DEQs (equations 2, 6, 9, and 15). In this model, each stream zone is discretized into 400 subzones. Within each subzone, Q is allowed to vary with distance x, but only linearly. The average velocity for the subzone $\overline{u}_\mathrm{sz}$ (m/s) thus is computed as the velocity at the subzone starting point. The overall time interval for integration over each subzone is determined as $\Delta x_\mathrm{sz}/\overline{u}_\mathrm{sz}$, where Δx_sz (m) is the length of the subzone. The final c_i and $\alpha_{i,j}$ values from the integration over a given subzone serve as the initial values for the next subzone.

A large change in flow over a subzone (with or without i) can cause instability in the numerical integration of equations 2, 6, 9, and 15. Therefore, StreamVOC distributes each point-source flow over a stream length, Δx_ps, equal to the minimum of the local stream width w or 5 m. Each point-source flow thus begins at zero at the upstream end of Δx_ps, is constant over the distance defined by Δx_ps, then decreases back to zero at the downstream end of Δx_ps. The total flow added over Δx_ps equals the flow of the point source. StreamVOC treats the change in flow due to a distributed ("nonpoint") source (or sink) flow that acts over a stream interval much larger than w (or 5 m) in an identical manner, where the differential change in flow is constant over the source region.

The effect of weirs and spillways on VOC concentrations and their SAs was calculated as described previously using equations 16–20 and 37–43. StreamVOC treats the decrease or increase in c_i as an instantaneous event that happens at the end of the subzone containing the hydraulic structure. Under this assumption, the concentration calculated at the end of a subzone containing a hydraulic structure is modified according to the equations described previously. In the case of VOC transfer from the atmosphere to the water at the structure, the source apportionments also are changed instantaneously. These new values are then used to initialize the Runge-Kutta algorithm at the start of the next subzone.

User Instructions and Information Needs for Running StreamVOC

StreamVOC has been tested using Microsoft Windows 9x, Windows NT 4.0, and Windows 2000/XP. It can be installed to run using a shortcut from the desktop, double clicking on the file StreamVOC.exe in Windows Explorer, or from the Start/Program/Run menu. Apart from copying the executable file to a particular location, no other installation steps are required for StreamVOC.

The data used to initialize and run StreamVOC are entered through an ASCII parameter file, an example of which for modeling methyl *tert*-butyl ether (MTBE) in a 4-km-long section of a hypothetical stream is shown in figure 2. The menu item for reading a parameter file is found under the File menu heading. StreamVOC cannot be run until an error-free parameter file has been read in through the File menu.

The general structure of the parameter file is given in an explanatory comment line that serves as a reminder to the user of the data required and its format followed by one or more lines of input data. The parameter file may be generated using any ASCII-based text editor. In general, word processors should not be used to generate the parameter files due to the presence of embedded codes and non-ASCII text format in the resulting file.

The first two lines of the parameter file set values for three flags related to the operation of StreamVOC. The first flag determines whether the model uses the net flux method or the component flux method to calculate the atmospheric SA term (flag = 0 will cause model to use net flux method, flag = 1 will cause model to use component flux method). The second flag determines whether or not there is water flowing under hydraulic structures (flag = 0 means no water flowing hydraulic structures, flag = 1 will have 20 percent of flow going under hydraulic structures). The third flag instructs the model to expect that streamflow values will be entered in units of cubic meters per second (flag = 0) or cubic feet per minute (flag = 1). The values of these flags must be either zero or one, all three must be present, and their order is not interchangeable.

The next six lines of the parameter file contain the total stream length L (km), the number of zones, and the number of distributed sources/sinks. Zone boundaries are defined as locations where there are point sources of VOCs, tributaries, changes in river depth h (m), changes in river width w (m), or changes in streamflow ΔQ (m^3/s). The next section of the parameter file contains the stream physical data in tabular form. The first line in the table gives the initial stream conditions. Subsequent lines of the table list the data for zone boundaries, point sources, or distributed source/sink regions. The structure of each line is Index Number, Start, Stop, h, w, ΔQ, and the VOC concentration in any sources (μg/L). In the case of a zone boundary or a point source, Start = Stop, and in the case of a distributed source, Start < Stop. Furthermore, the Stop location of a distributed source cannot be greater than the Start location of the subsequent zone boundary or distributed source (that is, distributed sources cannot overlap zone boundaries or other distributed sources).

In the example shown in figure 2, L = 4.000 km, and there are four zones and three distributed source regions in the stream. The first line of the stream physical data table shows that initially h = 0.30 m, w = 5.0 m, Q = 0.354 m^3/s, and c_i = 0.75 μg/L. The second line of the table shows that a distributed source starts at x = 0.000 km and continues until x = 1.000 km. The total flow added to the stream by this source is 0.035 m^3/s so that the rate of change of Q due to this source would be 0.035 m^3/s-km. Finally, the source has a VOC concentration of 1.25 μg/L. The third line shows the zone boundary between the first and second zones. At this boundary, h increases from 0.30 to 0.50 m, w increases from 5.0 to 8.0 m, and there is no change in Q. The fourth line is the zone boundary between the second and third zones. Here, h increases from 0.50 to 0.75 m with no change in either w or Q. The fifth line defines the second distributed source, which is an area of ground-water recharge as $\Delta Q < 0$. The sixth line defines the boundary between the third and fourth zones and shows that h decreases from 0.75 to 0.50 m with w remaining constant at 8.0 m. However, in contrast to the previous two zone boundaries, the boundary between the third and fourth zones also is a point source (or confluence) where there is a ΔQ of 0.189 m^3/s and an incoming VOC concentration in this flow of 2.50 μg/L. The eighth and final line in the stream physical data table is the end point of the stream to be modeled. The Start location in the final line must be equal to L, and the other data in this line are unused by StreamVOC.

In the case of distributed and point sources, ΔQ is allowed to be positive or negative. However, all other values in the physical data table must be greater than or equal to zero.

The 10 lines of the parameter file after the stream physical data table contain the environmental data for the stream, including water temperature T_w (°C), air temperature T_A (°C), mean wind speed U (m/s), relative humidity (percent), and local atmospheric (barometric) pressure P (atm). All five of these values are assumed to be constant over the entire stream.

Following the environmental data, the next 14 lines are used to enter the physicochemical data for the VOC to be modeled. The first data item for the VOC is its atmospheric concentration, f_i (ppbv), entered here as its atmospheric mixing ratio. The second item is the molecular weight of the VOC, MW_i (g/mol). Diffusivity is parameterized in StreamVOC using the molar volume-based relation of Wilke and Chang (1955). The molar volume of the VOC at its normal boiling point $\overline{V}_i$ (cm^3/mol), the fourth item, can be entered directly or it can be entered as the density of the liquid in grams per cubic centimeter on the flag in the third item. The aqueous-phase solubility of the VOC, the sixth item, is parameterized in terms of the Henry's Gas Law constant H_i (m^3-atm/mol). This can be entered in one of three ways indicated by the appropriate flag in the fifth item. First, it may be entered using the two-parameter exponential relation given in equation 36. Secondly, the five-parameter polynomial expression from Wanninkhof (1992) may be used. The third way is to calculate it externally from StreamVOC and enter that value directly. The final VOC physicochemical data item required is the biochemical degradation rate k_{deg} (l/s), which is optional and may be set to zero for no degradation.

The tolerance parameter for the Runge-Kutta routine is related to the precision of the answer. In general, the number of significant digits of the answer, N, can be selected by choosing the value of the tolerance to be equal to 10^{-N}. However, there is a limit to this relation so that at some point increasing N will have no appreciable effect on the answer. Users can verify that this is true by running StreamVOC successively with the tolerance set at 10^{-N} and 10^{-N-1}. If smaller values of the parameter produce no change in the model output, it may be assumed that further decreases will have no effect on model performance.

The next four lines are a parameter file header line and three lines of text that permit the user to annotate a particular model run with a title and as many as two lines of comments describing model conditions. There is a 72-character limit for the title and comment lines.

```
Flux method (0=Net, 1=Component):  Weir Flow (0=off, 1=on): Units (0=cubic meters per
second, 1=cubic feet per minute)
       1    0    0
Total Length of River (km)
       4.000
 Number of reaches
       4
 Number of distributed source regions
       3
 River profile/source data (# of points = # of reaches + # of distributed
sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0         0.30        5.0         0.354         0.75
 2    0.0          1.000       0.30        5.0         0.035         1.25
 3    1.000        1.000       0.50        8.0         0.0           0.00
 4    2.000        2.000       0.75        8.0         0.0           0.00
 5    2.000        3.000       0.75        8.0        -0.012         0.00
 6    3.000        3.000       0.50        8.0         0.189         2.50
 7    3.000        4.000       0.50        8.0         0.047         0.00
 8    4.000        4.000       0.50        8.0         0.047         0.00
River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       1.00
 Atmospheric VOC concentration (ppbv)
       0.5
 VOC molecular weight in g/mole
       88.15
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar Volume at B.P. (cm^3/mol) or density (g/cm^3)
       129.4
 Solubility param (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Solubility Coefficients mol/m^3-atm (1: D.E., 2: exp(A-B/T), 5: Wann.)
       0.184000E+02      0.766600E+04
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
      0.1000E-08
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2-1;~Sample~Parameter~File
Methyl-t-butyl-ether
This~line~for~additional~comments
waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;  2 = sharp-crested weir;  3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
  1         1.500        4.0      0.9        0.0              1.07            1
  2         3.250        4.0      0.5        0.0              0.64            2
d:\streamvoc\output_data\test1.dat
```

Figure 2. Sample ASCII parameter file used by StreamVOC.

The next section of the parameter file allows the user to enter the locations and types of any weirs, waterfalls, or hydraulic structures present in the stream. After two initial text lines that denote the beginning of the weir setup data entry, the first parameter is the number of weirs or structures. The weir number is followed by two more text lines, then the table containing the information for each structure in the stream. There must be one line in the table for each structure. The format of each line of the table is the structure index, the location of the structure from the beginning of the stream (km), the length of the structure (m), the height of the structure (m), the sill depth (m) if applicable, the tailstock depth (m) if applicable, and a numerical index defining the type of structure. As shown in figure 2, the Type index can take on the values 1 for an ogee-crested weir, 2 for a sharp-crested weir, and 3 for a gated spillway. The presence of the hydraulic structure portion of the parameter file is optional unless entry of the optional filename for model data output also is desired.

The final line in the parameter file is an optional filename for output of the model data. This option should be used with caution because if this filename is included in the parameter list, StreamVOC will overwrite any existing data file with the same name. Also, the user is responsible for ensuring that any directory path included with the filename is valid. If the user wishes to use this feature and there are no hydraulic structures in the stream, the parameter file must include the two text lines that start the hydraulic structure information portion, a line giving the number of hydraulic structures as zero, and the two text lines preceding the table containing the hydraulic structure information. Because there will be no entries in this table, the data output filename will follow immediately after these two lines of text. The output interval is one data point per subzone and cannot be altered by the user. Alternatively, the drive, directory, and file to which the data are written can be set by the 'Save VOC Model Results' option under the "File" menu in the main window of StreamVOC. If a model run is initiated without an output filename specified, the user will be notified that the results will not be saved to disk.

Inconsistencies or nonrealistic values (that is, VOC concentrations < 0) in the parameter file will be flagged in an error display window. The parameter file must be modified externally from StreamVOC to correct these errors and re-read into StreamVOC from the File/Read Parameter File submenu. Once a parameter file has been entered, the Run and View Parameters submenu options will be enabled. At this point, the input parameters may be examined in the model using the View Parameters menu options. Once it has been determined that the input information is correct, the model is started using the "Start Model" option under the "Run" menu in the main window. Model output to the main screen should begin soon after the run has been started. The user may terminate a model run before the final time using the "Halt Model" option in the "Run" menu. All other menu items are disabled while the model is running.

Verification of StreamVOC

The performance of StreamVOC was evaluated for numerical accuracy in two ways. First, numerical experiments were conducted using a hypothetical stream where the VOC concentration could be calculated analytically as a function of distance in a study region. By running different scenarios of point and distributed sources, the numerics of the model in regards to dilution, air-water gas exchange, and the SA calculations could be tested. The second set of experiments made use of a source synoptic study data set from the Aberjona River in Winchester, Massachusetts. This data set provided a means to test the performance of the model in estimating measured surface-water concentrations in a more realistic stream.

Hypothetical Base-Case Stream Using Methyl *tert*-Butyl Ether

The simulations described in this section were carried out using methyl *tert*-butyl ether (MTBE) as the VOC of interest to check the performance of the code. These tests involved a hypothetical base-case stream with $L = 100$ km, $w = 5$ m, $h = 0.5$ m, $u = 0.4$ m/s, $Q = 1$ m^3/s, $T_w = 20°C$, $P = 1$ atm, and $U = 4$ m/s (it should be noted that the example used here does not correspond to the parameter file shown in figure 2). The long and uniform nature of the stream allowed the gas exchange parameterization in the model to be tested by comparing the timescales required for achievement of Henry's Gas Law equilibrium between the stream and the atmosphere to timescales derived from analytical solutions of the relevant DEQs. Equation 36 with A_{MTBE} and B_{MTBE} from Robbins and others (1993) was used to determine that $H_{MTBE}(T_w = 20°C) = 4.3 \times 10^{-4}$ m^3-atm/mol. $\overline{V}_{MTBE}$ was based on density data (for liquid MTBE) found in the Beilstein CrossFire database BS030200PR at *http://chemistry.library.wisc.edu/beilstein/home.htm*. Sensitivity tests indicated that $k_{OL,i}$ depends only very weakly on wind velocity U for many VOCs, even for a relatively soluble VOC such as MTBE.

Mixing/dilution as performed in StreamVOC was examined using two test cases built on the base-case stream. The assumed water and air levels place the base-case stream initially supersaturated with respect to Henry's Gas Law equilibrium for MTBE. For both cases, the MTBE concentration in the inflow to zone 1 ($x = 0$) was assigned as 5.0 μg/L, and f_{MTBE} for the atmosphere was assigned as 5.0 ppbv. (For $H_{MTBE}(T_w = 20°C) = 4.3 \times 10^{-4}$ m^3-atm/mol, 5.0 ppbv corresponds to $c_{s,MTBE} = 1.0$ ppbv/(μg/L).) In the first test case, an MTBE-free point flow of 1 m^3/s was placed at $x = 1$ km. Immediately upstream from the added flow at $x = 0.9975$ km, the model simulated MTBE concentration = 4.986 μg/L; immediately downstream from the added flow at $x = 1.0005$ km, the model correctly simulated MTBE concentration = 2.493 μg/L. Because there was not enough distance over the point-source region for there to be an

appreciable loss of MTBE due to volatilization, MTBE decreased through dilution by a factor of two as expected. In the second test case, the point-source flow was replaced with a 1 m^3/s MTBE-free distributed flow that extended from $x = 1$ km to 2 km. At $x = 0.9975$ km, the model simulated MTBE concentration = 4.986 µg/L; at $x = 2.000$ km, the model simulated MTBE concentration = 2.488 µg/L. In this second case, the loss of MTBE through volatilization over the 1-km-long source region causes a small, but noticeable, decrease in MTBE that is in addition to the much larger decrease by dilution. Therefore, the final concentration is less than in the previous example although still approximately a decrease of a factor of two.

SA allocations for the net flux method as performed by StreamVOC also were examined using two test cases built on the base-case stream, and using the same inflow ($x = 0$) water concentration (MTBE concentration = 5.0 µg/L), and the same air level ($f_{MTBE} = 5.0$ ppbv) utilized in the two mixing/dilution test cases. In the first SA test, an added point-source (PS) flow of 1 m^3/s with MTBE concentration = 5 µg/L was located at 1 km. Immediately upstream from the point source, Stream-VOC estimated MTBE concentration = 4.986 µg/L with $\alpha_{INFLOW} = 1.0$ and $\alpha_{PS} = 0.0$; immediately downstream from the point source, the model estimated MTBE concentration = 4.992 µg/L with $\alpha_{INFLOW} = 0.4994$ and $\alpha_{PS} = 0.5006$. Neglecting volatilization losses and accounting only for mixing, the values calculated for MTBE concentration, α_{INFLOW}, and α_{PS} were 4.992 µg/L, 0.4993, and 0.5007, respectively. In a second SA allocation test, the added source acting along the stream was changed to a distributed flow, nonpoint source (NPS) extending from $x = 1$ to 2 km, with 1 m^3/s of total added flow, and MTBE concentration = 5.0 µg/L in that flow. At $x = 1$ km, the model estimated MTBE concentration = 4.986 µg/L, $\alpha_{INFLOW} = 1.0$, and $\alpha_{NPS} = 0.0$. At $x = 2$ km, the model correctly estimated MTBE concentration = 4.983 µg/L, $\alpha_{INFLOW} = 0.4991$, and $\alpha_{NPS} = 0.5009$. The slightly larger α value for the NPS resulted from proportionally more volatilization of the inflow-related MTBE than of the NPS-related MTBE.

SA calculations for the component flux method were tested by observing that when the aqueous-phase VOC concentration is in equilibrium with the atmosphere and the initial source fraction for the atmospheric source is zero, the time evolution of $\alpha_{i,air}$ has the closed-form analytical solution

$$\alpha_{i,air} = 1 - \exp\left(-\frac{k_{OA,i}t}{h}\right). \tag{45}$$

Figure 3 shows $\alpha_{i,air}$ calculated by StreamVOC for a stream having the physical characteristics described previously that is in equilibrium with an atmospheric concentration of MTBE of 5 ppbv. Figure 3 also shows $\alpha_{i,air}$ calculated using the analytical solution in equation 45. There is no substantial difference between the model output and the analytical solution.

Gas transfer as performed in StreamVOC was examined using two test cases built on the base-case stream and the same air level ($f_{MTBE} = 5.0$ ppbv) used previously. For the first test case, the stream was assumed to contain MTBE concentration at 5.0 µg/L at $x = 0$. Volatilization to the atmosphere would thus

tend to occur until MTBE dropped to 1.005 µg/L; the model simulated MTBE concentration = 1.006 µg/L at $x = 83.208$ km, which is consistent with that expectation. For the second test case, the stream inflow ($x = 0$) was assumed to contain MTBE concentration at 0.1 µg/L. Ingassing from the atmosphere would thus tend to occur until MTBE concentration = 1.005 µg/L; the model simulated MTBE concentration = 1.005 µg/L at $x = 70.677$ km.

The in-stream loss as calculated by StreamVOC was examined by addition of degradation (with $k_{deg,MTBE} = 2 \times 10^{-5}$/s) to the two gas-transfer test cases considered previously. Because f_{MTBE} in the atmosphere is not zero for these two cases, the inclusion of constant degradation means that Henry's Gas Law equilibrium can never be reached for either case, even at very large x. However, at sufficiently large x, the stream can achieve a steady-state condition for which the local MTBE entry rate into the river balances the local in-stream loss rate by degradation. For the case when the initial MTBE concentration = 5 µg/L, the model simulated a steady-state MTBE concentration of 0.6660 µg/L for $x > 80.2$ km. For a parcel of water corresponding to 1 second's worth of flow, the corresponding MTBE entry and loss rates are both 1.33 µg/L-s. For the case when the initial MTBE concentration = 0.1 µg/L, the same steady-state condition was reached once $x > 60.150$ km.

The concentrations of MTBE estimated by StreamVOC for the gas exchange test cases described previously can be further evaluated by comparison to the analytical solution of the DEQ for the test system. Because the stream for the validation studies had $m_{in,i} = 0$, $\Phi_{gw} = 0$, and constant Q, u, and h, integration of equation 2 shows that the concentration at any point x in the stream, $c_i(x)$, is given by

$$c_i(x) = \frac{k_{OL,i}c_{s,i}}{k_{OL,i} + hk_{deg,i}} - \left(\frac{k_{OL,i}\,c_{s,i}}{k_{OL,i} + hk_{deg,i}} - c_{0,i}\right)x$$

$$\exp\left[-\left(\frac{k_{OL,i}}{h} + k_{deg,i}\right)\frac{x}{u}\right], \tag{46}$$

where c_0 is the VOC concentration at the upstream end of the stream. The stream physical conditions used are $L = 100$ km, $w = 5$ m, $h = 0.5$ m, $u = 0.4$ m/s, $Q = 1$ m^3/s, $T_w = 20°$C, $P = 1$ atm, and $U = 4$ m/s. From these values, direct calculation of $k_{OL,MTBE}$ using the relations in the Physicochemical Parameterizations section found $k_{OL,MTBE} = 1.963 \times 10^{-5}$ m/s, which is identical to the numerical value produced by StreamVOC.

Figure 4 shows the model simulated MTBE concentration plotted along with the analytical solution shown in equation 46 for air-water transfer with no biochemical degradation (that is, $k_{deg,i} = 0$) for $c_0 > c_s$ (outgassing) and $c_0 < c_s$ (ingassing). The model results match the analytical solution to the fourth decimal place, which demonstrates that StreamVOC is correctly calculating the air-water exchange of VOCs for both invasion and evasion when there is no biochemical degradation.
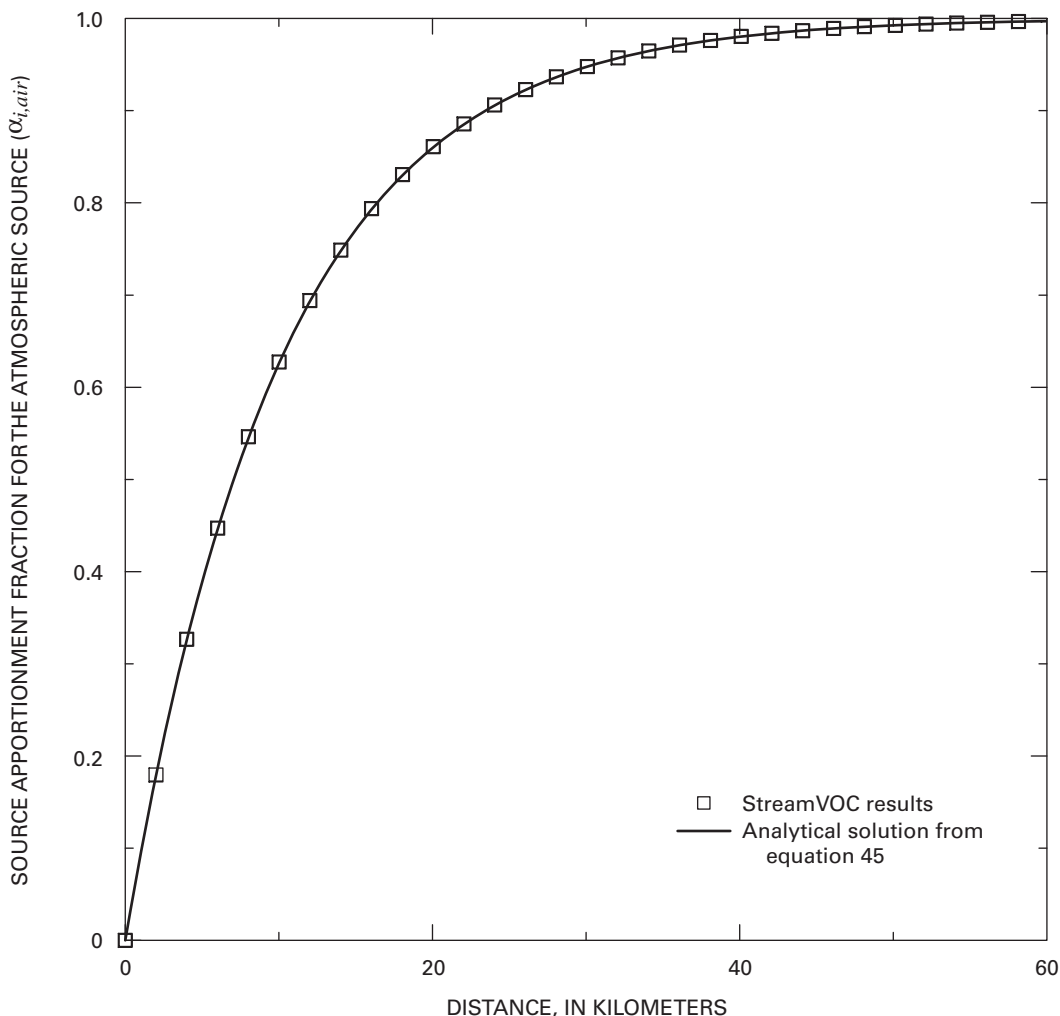
Figure 3. Source apportionment fraction for the atmospheric source, $\alpha_{i,air}$, of methyl *tert*-butyl ether calculated by StreamVOC for a stream in atmospheric equilibrium using the component flux method for the test stream described in text. Also shown are values for $\alpha_{i,air}$ calculated using the analytical solution given in equation 45 for the same conditions as used in the model.

Figure 5 shows the model simulated MTBE concentration plotted along the analytical solution shown previously for air-water transfer with $k_{deg,MTBE} = 2 \times 10^{-5}$/s for $c_0 > c_s$ (evasion) and $c_0 < c_s$ (invasion). The model results when degradation is included as a VOC loss mechanism also match the analytical solution to the fourth decimal place. The comparisons shown in figures 4 and 5 and discussed in this section demonstrate that the numerical solutions of StreamVOC function correctly.

StreamVOC Validation Using the Aberjona River

The performance of StreamVOC in modeling concentrations and their SAs in an actual stream was tested using a data set collected on the Aberjona River in Winchester, Massachusetts, for an intensive source-synoptic study during July 11–13, 2001. This section of the report describes the test site and provides modeling results for eight VOCs.

Study Test Site Description

Depth (h), width (w), and flow (Q) values were measured over a 2.811-km section of the stream on July 11, 2001. Figure 6 and table 1 show that the 2.811-km section was divided into 10 main zones based on stream characteristics. Zone 8 contains two ponds connected by a short channel, and in terms of model parameterization, each pond and the connecting channel were defined as separate subzones in zone 8. The confluence with Horn Pond Brook is located immediately upstream from the boundary between zones 7 and 8a, and for convenience of discussion in this report this confluence is considered to coincide with the zone boundary. The stream zone numbers and distance increase going downstream. Figure 7 shows the average values for u calculated from h, w, and Q; Q determined from flow measurements; and w and h in each zone plotted as a function of distance downstream from the start of the synoptic study
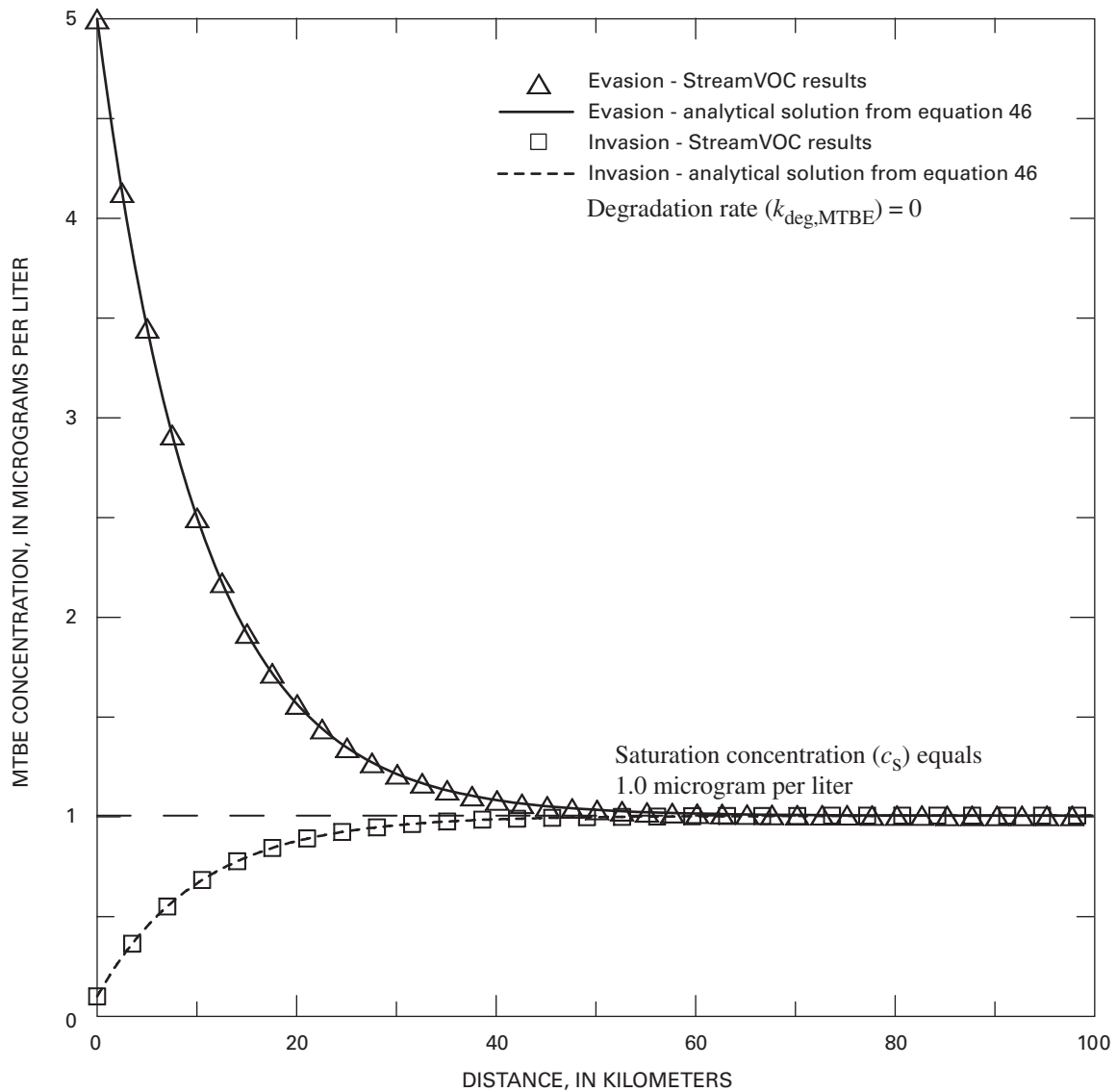
Figure 4. Concentration of methyl *tert*-butyl ether (MTBE) calculated by StreamVOC assuming no biochemical degradation for the test stream described in text. Also shown are MTBE values calculated using the analytical solution of equation 2 given in equation 46 for the same conditions as used in the model.

region. The presence of the ponds in zones 8a and 8c reduces u in these sections to less than 0.04 m/s, and the air-water gas exchange is then driven by wind stress as shown by equation 29.

The hydrogeologic setting of the Aberjona River watershed is typical of what is found in glaciated areas of southern New England—a gentle valley underlain by bedrock and surficial till, sand, and gravel deposits (deLima and Olimpio, 1989). A sand and gravel aquifer is present along the stream course and tapers outward along the slopes of the surrounding hills. North of Winchester in Woburn, Massachusetts, the thickness of this aquifer ranges from zero at the sides of the valley to 140 ft underneath the stream channel (deLima and Olimpio, 1989). This aquifer contains layers ranging from fine sands and silt to course sands and gravels. Peat deposits also are adjacent to and underneath the Aberjona River in some locations. A layer of till is beneath the sand and gravel aquifer and is present on the surface where the sand and gravel deposits are absent. Bedrock outcrops are along the slopes and tops of the valley divide. Ground-water flow generally is downgradient along the valley sides towards the river; the river is a discharge point of ground water. There also is vertical mixing of ground water within the sand and gravel aquifer and between the surficial and bedrock aquifers.

When possible, h and w were measured at multiple locations in a zone across the stream in the case of h and along the stream in the case of w. Q was measured at the end of each zone and tracked over the duration of the synoptic study. Surface-water samples were collected on July 11, 2001, between the hours of 0600 Eastern Daylight Time (EDT) and 2000 EDT, during which Q decreased from 0.680 to 0.596 m^3/s with a time-weighted average of 0.613 m^3/s.
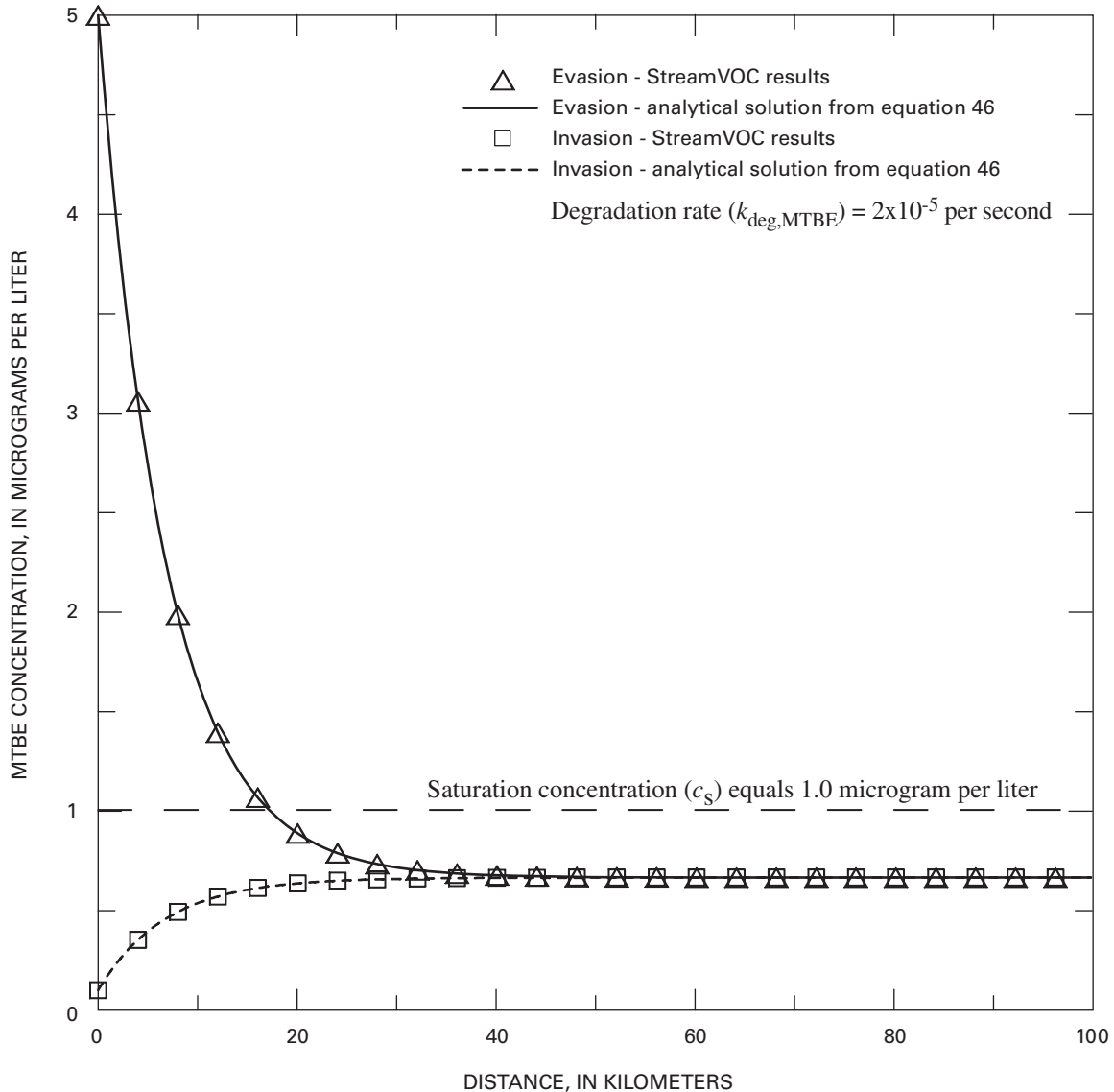
Figure 5. Concentration of methyl *tert*-butyl ether (MTBE) calculated by StreamVOC assuming a biochemical degradation rate of 2×10^{-5} per second for the test stream described in text. Also shown are MTBE values calculated using the analytical solution of equation 2 given in equation 46 for the same conditions as used in the model.

There are two hydraulic structures in the Aberjona River in the synoptic study region, and their locations are denoted at the top of figure 7. In order of zone number, the first structure is located at the downstream end of zone 8c and is a small stepped dam that was assumed to function like a sharp-crested spillway in terms of its air-water exchange characteristics. The second structure is an ogee-crested weir located at the downstream end of zone 9. The dimensions of the dam and weir used in calculating their respective $E_i(H_i)$ values were determined from photographs taken during the synoptic study measurements. Stream-water samples were collected downstream from both the dam in zone 8c and the weir in zone 9, a detail that will have relevance when interpreting the modeling results presented later.

Surface-water samples were obtained at a single point in the centroid of flow by the grab-sampling technique using VOC sampling methods described in published NAWQA guidelines (Mueller and others, 1997; Shelton, 1997). Ground-water samples were obtained using a 1-in. diameter drive point installed in the center of the streambed channel to a depth of approximately 1 m below the streambed. The drive point was purged during installation three to four times to remove foreign matter and allowed to stabilize for approximately 8 hours prior to sampling. The drive point was purged of three volumes of water and then sampled using a peristaltic pump and clean Teflon tubing. Sampling positions were determined using a global positioning
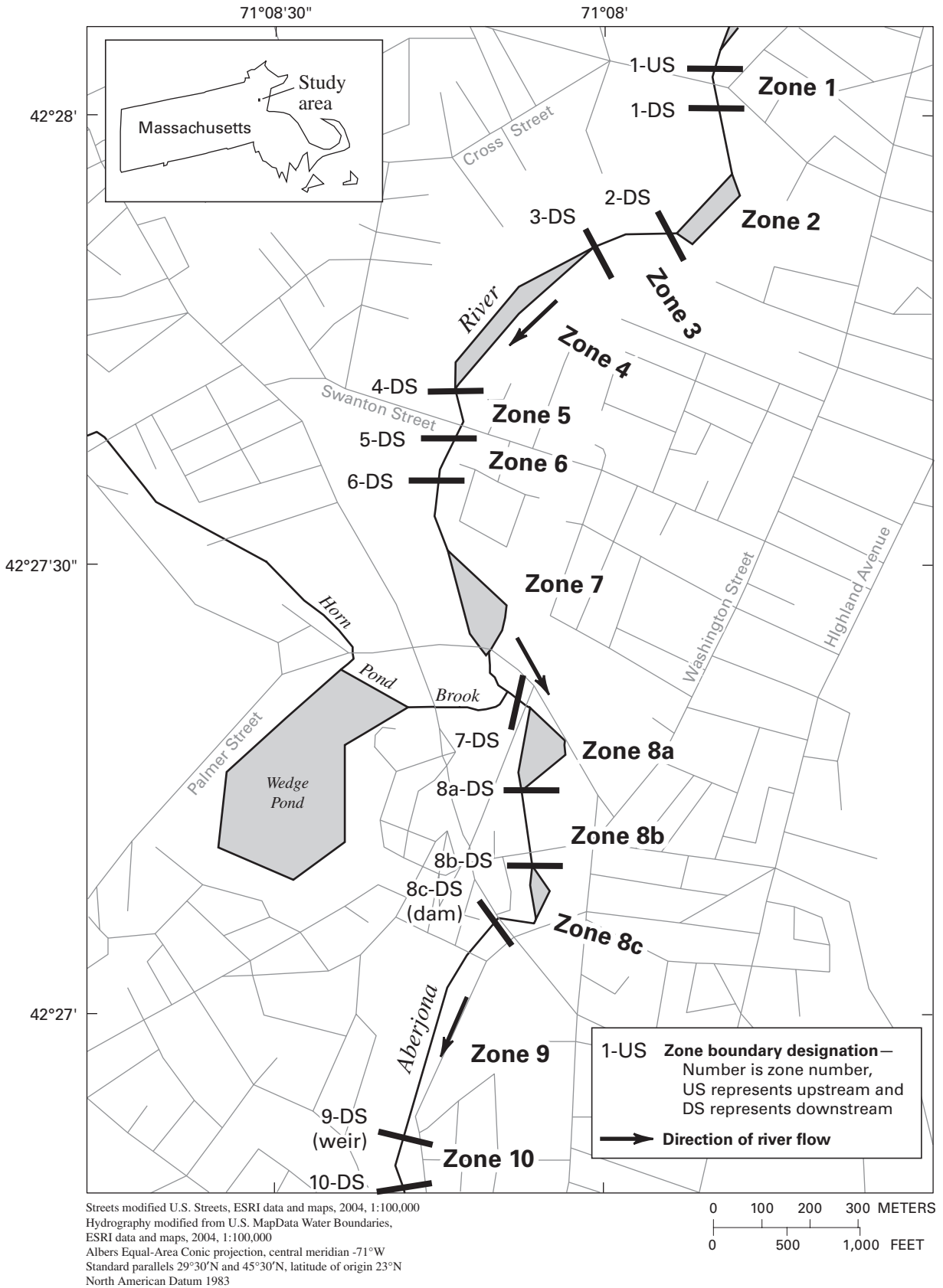
Figure 6. Study section of Aberjona River (Winchester, Massachusetts) showing locations of the 10 stream zones and the confluence with Horn Pond Brook.

Table 1. Synoptic data for Aberjona River system, July 11–13, 2001.

[km, kilometers; m, meters; m^3/s, cubic meter per second; NA, not available]

Zone (see fig. 6)	Upstream zone boundary (km)	Downstream zone boundary (km)	Average stream width (w) (m)	Average stream depth (h) (m)	Streamflow at upstream end of zone (Q) (m^3/s)	Change in stream-flow due to ground water ($\triangle Q$) (m^3/s)
			Aberjona River			
1	0	0.096	5.5	0.30	0.354	0.0368
2	.096	.400	7.3	.53	.3908	.0227
3	.400	.540	7.9	.76	.4135	.0925
4	.540	1.090	22.8	.34	.5060	-.173
5	1.090	1.150	8.5	.64	.3330	.0538
6	1.150	1.230	7.3	.79	.3868	-.0595
7	1.230	1.647	3.6	.37	.3273	-.0264
8a	1.647	1.897	100.0	2.0	.3009	.0156
8b	1.897	2.147	10.0	2.0	.5185	0
8c	2.147	2.293	90.0	2.0	.5185	.0118
9	2.293	2.736	10.7	1.07	.5303	.0311
10	2.736	2.811	7.9	.64	.5614	.0510
Horn Pond Brook	1.647	1.647	NA	NA	.202	NA

system (GPS) device. Surface-water and ground-water drive-point sample collection occurred at the 12 locations defining the upstream boundary of zone 1 and the downstream boundaries of zones 1, 2, 3, 4, 5, 6, 7, 8b, 8c, 9, and 10 shown in figure 6. Surface-water samples also were collected from the main tributary, Horn Pond Brook, at a point immediately upstream from its confluence with the river. Water concentrations of 87 VOCs were determined at the Oregon Health and Science University, Department of Biomolecular Systems Laboratory, using a method previously published by Connor and others (1998). The 87 VOCs also were determined from 10-hour composite air samples obtained at the centroid of the source-synoptic study area; the air analytical method utilized is described in detail by Pankow and others (1998).

Out of 87 total VOCs sampled, 8 compounds listed in tables 2–4 (acetone, benzene, MTBE, chloroform, 1,1-dichloroethane (1,1-DCA), cis-1,2-dichloroethene (cis-1,2-DCE), trichloroethene (TCE), and perchloroethene (PCE, also known as tetrachloroethene)) were found with sufficient spatial coverage in the Aberjona River system to allow meaningful comparison of the measured data with model results produced by StreamVOC. The method detection limit (MDL) values for the eight compounds were as follows: acetone = 0.67 μg/L; benzene = 0.014 μg/L; MTBE = 0.025 μg/L; chloroform = 0.017 μg/L; 1,1-DCA = 0.011 μg/L; cis-1,2-DCE = 0.013 μg/L; TCE = 0.020 μg/L; and PCE = 0.027 μg/L. In general, the MDLs are higher than the typical instrumental detection limits. Because of this, it is possible for the analysis to show that a VOC is qualitatively present in a sample even though its concentration is below the MDL. In those cases, the VOC

concentration was estimated by assuming a linear response and extrapolated using the lowest available standard for that day. In tables 2–4, an entry of ND denotes that the VOC was not qualitatively present in the sample, indicating that the concentration either was below the instrumental detection limit or was in fact zero. No attempt was made to distinguish between these two cases, and we have arbitrarily assumed a zero value for the concentration of any VOC that was listed as ND.

Replicate surface-water samples collected at the downstream end of zone 5 showed the following percent differences between the two concentrations: acetone, 58 percent; benzene, not detected (ND); MTBE, 11 percent; chloroform, 8.3 percent; 1,1-DCA, 15 percent; cis-1,2-DCE, 4.0 percent; TCE, 0 percent; and PCE, 27 percent (table 2). Replicate ground-water samples were collected at the downstream end of zone 1 and the downstream end of zone 10. The percent differences between these replicate samples where the VOC was detected were: acetone (zone 1), 0.6 percent; MTBE (zone 1), 6.1 percent; chloroform (zone 10), 14 percent; 1,1-DCA (zone 1), 6.2 percent; cis-1,2-DCE (zone 1), 16 percent; and TCE (zone 1), 12.5 percent (table 3).

The $c_{s,i}$ values in table 4 were calculated using the measured atmospheric concentrations and H_i values obtained as follows: acetone from Zhou and Mopper (1990); benzene from Leighton and Calo (1981); chloroform, 1,1-DCA, cis-1,2-DCE, and PCE from Gossett (1987); MTBE from Robbins and others (1993); TCE from Ashworth and others (1988). Values of $\overline{V}$ were based on density data found in the Beilstein Crossfire online database BS030200PR at *http://chemistry.library.wisc.edu/beilstein/home.htm*.
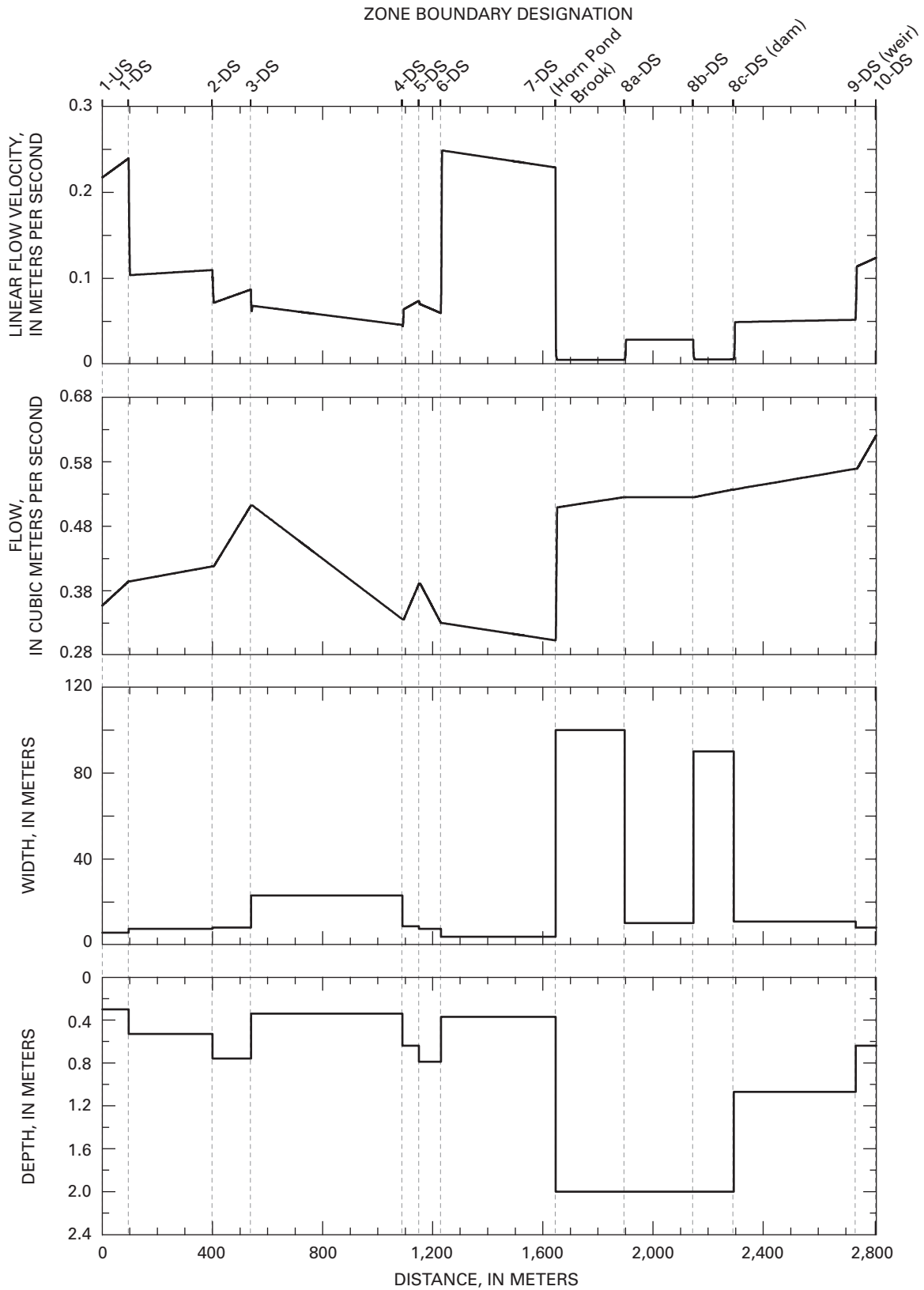
Figure 7. Physical characteristics of the Aberjona River as a function of distance where distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for zone locations). Intervals over which flow decreases represent intervals where streamflow is being lost to ground water, and intervals over which increases represent areas where ground water is discharging to the river or where tributaries flow into the river.

Table 2.   Volatile organic compound (VOC) concentrations in surface-water samples obtained during a synoptic study of the Aberjona River conducted July 11–13, 2001.

[µg/L, micrograms per liter; km, kilometers; US, upstream end; DS, downstream end; HPB, Horn Pond Brook; ND, not detected. No data were collected for zone 8a]

Zone sample point	Distance (km)	Concentration (µg/L)							
		Acetone C_3H_6O	Benzene C_6H_6	Methyl *tert*-butyl ether (MTBE) $C_5H_{12}O$	Chloroform $CHCl_3$	1,1-dichloro-ethane (1,1-DCA) $C_2H_4Cl_2$	*cis*-1,2-Dichloroethene (*cis*-1,2-DCE) $C_2H_2Cl_2$	Trichloro-ethene (TCE) C_2HCl_3	Perchloro-ethene (PCE) C_2Cl_4
1-US	0	0.56	0.009	0.61	0.12	0.038	0.3	0.17	0.039
1-DS	.096	.44	ND	.63	.12	.034	.26	.18	.048
2-DS	.400	.12	ND	.58	.12	.043	.23	.16	.1
3-DS	.540	.45	ND	.58	.12	.037	.26	.15	.1
4-DS	1.090	.4	ND	.4	.1	.091	.23	.21	.14
5-DS-A[1]	1.150	.38	ND	.54	.12	.096	.25	.32	.15
5-DS-B[2]	1.150	.6	ND	.48	.11	.11	.26	.32	.19
6-DS	1.230	.58	.007	.34	.092	.095	.23	.31	.14
HPB	1.647	ND	.05	4.12	ND	ND	.032	.035	ND
7-DS	1.647	.43	ND	.54	.1	.086	.23	.32	.13
8b-DS	2.147	.46	.019	.99	.07	.062	.15	.18	.074
8c-DS	2.293	.48	.009	.8	.072	.046	.12	.18	.16
9-DS	2.736	.086	.01	1.43	.08	.051	.14	.16	.19
10-DS	2.811	.15	.012	1.36	.071	.045	.12	.16	.18

[1]A = first sample.

[2]B = second (replicate) sample.

Table 3.   Volatile organic compound (VOC) concentrations in ground-water samples obtained during a synoptic study of the Aberjona River conducted July 11–13, 2001.

[km, kilometers; µg/L, micrograms per liter; US, upstream end; DS, downstream end; ND, not detected. No data were collected for zone 2]

Zone sample point	Distance (km)	Concentration (µg/L)							
		Acetone C_3H_6O	Benzene C_6H_6	Methyl *tert*-butyl ether (MTBE) $C_5H_{12}O$	Chloroform $CHCl_3$	1,1-Dichloro-ethane (1,1-DCA) $C_2H_4Cl_2$	*cis*-1,2-Dichloro-ethene (*cis*-1,2-DCE) $C_2H_2Cl_2$	Trichloro-ethene (TCE) C_2HCl_3	Perchloro-ethene (PCE) C_2Cl_4
1-US	0	0.15	ND	1.05	ND	ND	0.30	0.15	ND
1-DS-A[1]	.096	1.80	ND	.33	ND	0.48	.25	.24	ND
1-DS-B[2]	.096	1.79	ND	.35	ND	.51	.21	.21	ND
3-DS	.540	ND	ND	ND	1.16	ND	ND	.39	0.82
4-DS	1.090	.29	ND	ND	ND	ND	ND	.15	ND
5-DS	1.150	.43	ND	ND	ND	.12	.12	1.09	ND
6-DS	1.230	1.51	ND	3.17	ND	18.27	8.41	1.41	ND
7-DS	1.647	.44	ND	ND	ND	.29	.24	1.42	ND
8c-DS	2.293	.99	ND	ND	ND	ND	ND	ND	ND
9-DS	2.736	.61	ND	1.36	ND	ND	.33	ND	ND
10-DS-A[1]	2.811	ND	ND	ND	.35	ND	ND	ND	ND
10-DS-B[2]	2.811	ND	ND	ND	.40	ND	ND	ND	ND

[1]A = first sample.

[2]B = second (replicate) sample.

Table 4. Volatile organic compound (VOC) levels in air, water in equilibrium with that air, and in local stream water obtained during a synoptic study of the Aberjona River conducted July 11–13, 2001.

[km, kilometers; ppbv, parts per billion by volume; μg/L, micrograms per liter; MP, midpoint of zone; US, upstream end; DS, downstream end; ND, not detected]

Zone sample point	Distance (km)	Concentration							
		Acetone C_3H_6O	Benzene C_6H_6	Methyl *tert*-butyl ether (MTBE) $C_5H_{12}O$	Chloroform $CHCl_3$	1,1-Dichloro ethane (1,1-DCA) $C_2H_4Cl_2$	*cis*-1,2-Dichloro-ethene (*cis*-1,2-DCE) $C_2H_2Cl_2$	Trichloro-ethene (TCE) C_2HCl_3	Perchloro-ethene (PCE) C_2Cl_4
Measured air levels (ppbv)									
7-MP	1.44	0.69	0.20	0.26	0.045	ND	ND	0.014	0.073
Calculated equilibrium (Henry's Gas Law) stream-water concentrations (μg/L)									
7-MP	1.44	0.91	0.0032	0.044	0.0017	0	0	0.00020	0.00081
Measured stream-water concentrations (μg/L)									
7-US	1.23	0.58	0.007	0.34	0.092	0.095	0.23	0.31	0.14
7-DS	1.65	.43	ND	.54	.10	.086	.23	.32	.13
Stream status in zone 7—ingassing or outgassing									
7-US		ingassing[1]	outgassing[2]	outgassing	outgassing	outgassing	outgassing	outgassing	outgassing
7-DS		ingassing	undetermined[3]	outgassing	outgassing	outgassing	outgassing	outgassing	outgassing

[1]Ingassing = ingassing because the measured stream-water concentration is lower than the calculated equilibrium water concentration.

[2]Outgassing = outgassing because the measured stream-water concentration is higher than the calculated equilibrium water concentration.

[3]Undetermined = undetermined because the calculated equilibrium concentration is lower than the water method detection limit used to measure the stream-water concentration.

Over the entire Aberjona River synoptic study region, only acetone was undersaturated in the surface water with respect to its Henry's Gas Law equilibrium concentration. The other seven compounds were present at water concentrations that were supersaturated relative to the levels specified by equilibrium with the atmospheric levels measured in the vicinity of zone 6. In other words, the various c_i values from zones 1 through 10 for these seven VOCs were larger than the corresponding values of $c_{s,i}$ calculated based on the f_i values. It was therefore concluded that: (1) the river was probably losing all seven compounds by volatilization over the entire study interval; and (2) for the water flowing into zone 1, the local atmosphere probably was not the origin of the majority of any of the initial seven c_i values. Because the origins of the contaminants in the flow entering zone 1 are not known, for any stream point (x,t), the fraction of c_i due to the flow that entered zone 1 was arbitrarily assigned in this study to α_{INFLOW}.

In similarity with the other seven VOCs, the mass of acetone entering zone 1 was assigned to α_{INFLOW}. In contrast with a VOC where the surface water is supersaturated with respect to Henry's Gas Law, an unknown fraction of α_{INFLOW} for acetone

should more correctly be assigned to the atmospheric source fraction, α_{AIR}. However, without detailed information concerning the sources and surface-water concentrations of acetone upstream from zone 1, determining the fraction of α_{INFLOW} that should be assigned to the atmospheric source was not possible. Therefore, α_{INFLOW} for acetone was not partitioned into atmospheric and other source fractions.

The synoptic data were used with StreamVOC in model runs for the eight VOCs as follows. For each VOC, the model was initialized using the concentration measured in the stream-flow entering zone 1. After assuming that the regional air was sufficiently well mixed to allow the values of f_i and $c_{s,i}$ obtained for zone 6 to be applicable from zones 1 through 10, gas transfer across the stream/air interface was calculated to occur according to the previous equations. Modeled sources to the stream included calculated inflows to the stream from ground water, the point source from Horn Pond Brook, and the atmosphere in the case of acetone. Modeled losses included calculated outflows from the stream to ground water and outflow to the atmosphere in the case of benzene, MTBE, chloroform, 1,1-DCA, *cis*-1,2-DCE, TCE, and PCE.

Table 5. Chemical degradation half-lives ($\tau_{0.5}$).

[N.S., not significant based on relevant rates]

Compound	$\tau_{0.5}-$ Hydrolysis (years)	$\tau_{0.5}-$ Photolysis (years)	$\tau_{0.5}-$ Oxidation (years)
acetone	N.S.[1]	N.S.[1]	N.S.[1]
benzene	N.S.[2]	N.S.[2]	[2]0.92
methyl *tert*-butyl ether	N.S.[1]	N.S.[1]	N.S.[1]
chloroform	[2]1,800	N.S.[2]	[2]78
1,1-dichloroethane	[2]58	N.S.[2]	[2]100,000
cis-1,2-dichloroethene	[2]2.1×10^{10}	N.S.[1]	N.S.[1]
trichloroethene	[2]1.66×10^5	N.S.[2]	[2]10,000
perchloroethene	[2]9.56×10^8	N.S.[2]	[2]10,000

[1]U.S. Agency for Toxic Substances and Disease Registry, Toxicological Profile Sheet, *http://www.atsdr.cdc.gov/toxpro2.html*.

[2]Rathbun (2000).

Considerations of inflow and outflow from ground water in each zone made use of three assumptions: (1) inflow/outflow could be determined based on the difference in Q values measured at the zone endpoints; (2) inflow/outflow could be distributed uniformly over a given zone; and (3) when an inflow contained a VOC, the inflow concentration over the zone could be taken as being constant and equal to the value measured at the end of the zone by drive-point sampling. Compared to assigning the average zone inflow VOC concentrations to the ground-water concentration measured for that start point of that zone or assigning the average zone inflow VOC concentrations to the mean of the start point and endpoint ground-water concentrations, assigning the average zone inflow concentration as described in the third assumption gave the best overall fit between the model-simulated and measured surface-water VOC concentrations. Using zone 3 as an example of the implementation of the first assumption, Q was 0.414 m^3/s at the upstream end and 0.506 m^3/s at the downstream end. With no tributaries in this zone, the total inflow of ground water over zone 3 was 0.092 m^3/s. Using the data in table 3, the VOC concentrations in the ground-water inflows to zone 3 are acetone = 0.0 μg/L, benzene = 0.0 μg/L, MTBE = 0.0 μg/L, chloroform = 1.16 μg/L, 1,1-DCA = 0.0 μg/L, *cis*-1,2-DCE = 0.0 μg/L, TCE = 0.39 μg/L, and PCE = 0.82 μg/L.

Typical chemical degradation half-lives, $\tau_{0.5,i}$, for the eight VOCs considered for this model test are listed in table 5 for hydrolysis, photolysis, and oxidation in aqueous media. The half-life for each compound is defined in terms of its first-order rate constant, $k_{deg,i}$, where in the absence of volatilization, dilution, or other loss processes, the concentration of the VOC as a function of time is equal to

$$c_i = c_{i,0} e^{-k_{deg,i}t}, \qquad (47)$$

where $c_{i,0}$ is the concentration of i at $t = 0$. Therefore, $\tau_{0.5,i}$ is defined as $0.693/k_{deg,i}$. Typically, the values for $\tau_{0.5,i}$, when known, are on the order of years or longer. The total transit

time for a parcel of water in the source synoptic study region was approximately 52 hours. Given that this time is at least an order of magnitude smaller than the chemical degradation half-lives in table 5, chemical degradation is not likely to be important for these compounds.

Appendixes 2–1 through 2–8 list StreamVOC parameter files for the eight VOCs used in this study. The VOC sources were deduced from the synoptic study VOC concentration measurements. Appendix 3 gives the source synoptic input and output data for the eight VOCs used in this study, and Appendix 4 gives the physical and chemical properties.

Modeling Results

General

Figures 8–15 provide plots of the measured VOC concentrations obtained for the Aberjona River during the July 11–13, 2001, synoptic sampling. Also plotted are StreamVOC model results that simulate stream concentrations and corresponding SA fractions calculated using the net flux method based on (1) inputs determined from the synoptic-sampling effort; and (2) modified inputs derived from minimizing the reduced chi-square between the model-simulated and measured surface-water concentrations. In the case of (1), as described above, this means that in zones with ground-water inflow, the VOC concentration in the ground water was assigned to be equal to that measured during the source synoptic study, and the VOC concentration in Horn Pond Brook was taken to be that measured during the source synoptic study. In the case of (2), the ground-water inflow VOC concentrations and the VOC concentration in Horn Pond Brook were adjusted to minimize the reduced chi-square value between the model output and measured surface-water VOC concentrations. The reduced chi-square is defined as

$$\chi_i^2 = \sum_{k=1}^{N_{C,i}} \frac{\left(c_{i,k}^{ss} - c_{i,k}^{mod}\right)^2}{\left(c_{i,k}^{ss}\right)^2}, \qquad (48)$$

where χ_i^2 is the reduced chi-square optimization parameter for VOC i; $N_{C,i}$ is the number of non-zero surface-water concentrations measured during the source-synoptic study; $c_{i,k}^{ss}$ is the measured concentration of VOC i in zone k; and $c_{i,k}^{mod}$ is the model-simulated concentration of VOC i in zone k. Optimization of χ_i^2 was performed using the Solver.DLL nonlinear optimization package (Frontline Systems, Incline Village, Nevada). Table 6 gives χ_i^2 calculated using $c_{i,k}^{mod}$ derived from the source-synoptic inputs and the minimum value of χ_i^2 found by the optimization software. With the exception of acetone, the ratio of the initial to final χ_i^2 values shows that the optimization was highly significant statistically at the 99-percent confidence level. Table 7 lists the optimized VOC inputs that were found to minimize χ_i^2 between the measured and model-simulated surface-water VOC concentrations. StreamVOC parameter files for the eight VOCs used in this test model are shown in Appendixes 2–9 through 2–16.

Table 6. Reduced chi-square values calculated between the measured surface-water volatile organic compound (VOC) concentrations and concentrations estimated using the source synoptic VOC inputs and inputs optimized to minimize the reduced chi-square value, χ_i^2.

	χ_i^2							
	Acetone (ACE)	Benzene (BEN)	Methyl *tert*-butyl ether (MTBE)	Chloroform (CLF)	1,1-Dichloro-ethane (1,1-DCA)	*cis*-1,2-Dichloro-ethene (*cis*-1,2-DCE)	Trichloro-ethene (TCE)	Perchloro-ethene (PCE)
Source synoptic inputs	69	0.42	1.6	4.9	6.4	3.5	2.4	4.3
Optimized inputs	44	.032	.19	.066	.37	.037	.12	.21
Ratio	1.6	13	8.4	74	17	92	20	21

As noted previously, for each of the eight VOCs, α_{INFLOW} is the SA fraction corresponding to the portion of the VOC that entered the system at the upstream end of zone 1. Also, using the net flux method, because all of the VOCs except acetone were volatilizing over all 10 zones of the stream to the atmosphere, only the plots for acetone contain a non-zero value for the atmospheric source, α_{AIR}. For the other seven compounds, $\alpha_{AIR} = 0$ over all x and t using the net flux method. However, using the component flux method results in non-zero α_{AIR} for several other VOCs in addition to acetone.

Acetone

The synoptic sampling effort identified six sources of acetone for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1 (1-US), the atmosphere, and ground water entering zones 1, 5, 8c, and 9. The concentration of acetone as a function of distance in the study region calculated by StreamVOC using the acetone inputs derived directly from the source synoptic data is shown in figure 8*A* as the solid line. The SA calculations for the acetone inputs as determined directly from the data are shown in figure 8*B*.

The dashed line shown in figure 8*A* represents the Stream-VOC results from the model where the acetone concentrations in the ground water and Horn Pond Brook sources were adjusted to give the minimum value of χ^2 defined in equation 48 (table 7). In the case of acetone, this process determined that the best fit was obtained by setting all sources in the study region except the atmospheric source to zero. Figure 8*C* shows the SA calculations using the net flux method for the modified inputs, where only the initial source of acetone entering zone 1 and the atmospheric source are used.

As mentioned previously, acetone is the only VOC used in the study where $c_{s,acetone} > c_{acetone}$, implying that there is a net flux of acetone from the atmosphere into the stream water. The effect of this flux on the SA calculations is clearly seen in figure 8*B* and 8*C* as the atmospheric source fraction, α_{air}, increases in both cases from zero at the upstream end of zone 1 to approximately 45 percent at the downstream end of zone 10 for the source synoptic inputs in figure 8*B* and 65 percent for the optimized inputs in figure 8*C*. The effects of the dam at the downstream end of zone 8*C* and the weir at the downstream end

of zone 9 on acetone are seen as a step increase in $\alpha_{ACE,AIR}$ at both locations. In comparison to the other seven VOCs modeled and described in the following sections, the two structures have relatively little effect on acetone because it has the highest solubility and, therefore, lowest transfer efficiency, $E_{ACE}(H_{ACE})$.

Figure 8*D* shows the SA calculations using the component flux method for the source synoptic inputs. Because acetone is undersaturated and $\alpha_{ACE,AIR}$ is increasing even for the net flux method, the results are similar to the corresponding results in figure 8*B* except the final $\alpha_{ACE,AIR}$ value is larger. For the source-synoptic inputs, $\alpha_{ACE,AIR}$ is a little more than 75 percent at the downstream end of zone 10 using the component flux method compared with the 45 percent resulting from the net flux method.

Benzene

The synoptic sampling effort identified two sources of benzene for the Aberjona River study interval—the stream inflow to the study interval at the upstream end of zone 1 and Horn Pond Brook. The model-simulated benzene concentrations shown in figure 9*A* (solid line) and the SA calculations using the net flux method in figure 9*B* are based on model inputs from the synoptic sampling. The decreasing benzene concentrations over zones 1 through 6 (fig. 9*A*) are because $c_{BEN} > c_{s,BEN}$ throughout that range, and thus the stream loses benzene to the atmosphere. The same observation applies to the concentration trend observed over zones 8b through 10. The magnitude of the concentration increase between zone 6 and zone 8b is consistent with the increase estimated based on the benzene concentration and flow discharge of Horn Pond Brook, and there is good agreement between the measured and model-simulated concentrations in zones 6, 8b, and 8c. However, the measured and model-simulated concentrations diverge in zones 9 and 10 downstream from the two hydraulic structures.

Because H_i for benzene is a factor of 100 larger than for acetone, the weir transfer efficiency is much larger for benzene. This is reflected in the large drop in benzene concentrations at each of the two structures. However, following the theoretical discussion presented in the governing equations, there is no change in the SA because the river is outgassing VOC over the structures.

Table 7. Volatile organic compound (VOC) concentrations in Horn Pond Brook and ground-water inflows to the Aberjona River that minimize the reduced chi-square value between the measured and StreamVOC model-simulated surface-water VOC concentrations.

[μg/L, micrograms per liter, HPB, Horn Pond Brook; NC, no change]

| | Estimated concentration and concentration difference (μg/L) | | | | | | | | | | | | | | | |
| Zone | Acetone (ACE) | | Benzene (BEN) | | Methyl *tert*-butyl ether (MTBE) | | Chloroform (CLF) | | 1,1-Dichloroethane (1,1-DCA) | | *cis*-1,2-Dichloro-ethene (*cis*-1,2-DCE) | | Trichloroethene (TCE) | | Perchloroethene (PCE) | |
	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]	Concen-tration[1]	Differ-ence[2]
1	0	-1.79	0.012	0.012	0.92	0.58	0.19	0.19	0.0033	-0.48	0	-0.23	0.25	0.043	0.14	0.14
2	0	NC	.0084	.0084	.078	.078	.20	.20	.26	.26	0	NC	.14	.14	1.08	1.08
3	0	NC	.013	.013	.47	.47	.19	-.97	.047	.047	.54	.54	.26	-.13	.21	-.61
5	0	-.43	.0046	.0046	.71	.71	.26	.26	.55	.43	.68	.56	1.65	.56	.64	.64
HPB	0	NC	.054	.004	3.23	-.89	.16	.16	.13	.13	.33	.30	.34	.30	.091	.091
8c	0	-.99	0	NC	13.4	13.4	2.82	2.82	1.15	1.15	3.59	3.59	6.45	6.45	8.78	8.78
9	0	-.61	.03	.03	16.7	15.3	.56	.56	.36	.36	1.04	.71	.65	.65	1.53	1.53
10	0	NC	.038	.038	.73	.73	0	-.37	0	NC	0	NC	.19	.19	.11	.11

[1]Estimated source concentration (in μg/L) used to provide best match.

[2]Difference between source concentration used to provide best match and source concentration from the synoptic data set.

Figure 8. Acetone in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; *(C)* estimated SA values for sources chosen to provide best fit of acetone concentrations; and *(D)* estimated SA values calculated using the component flux method for sources determined by the source synoptic study data set. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).

Figure 9. Benzene in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; *(C)* estimated SA values for sources chosen to provide best fit of benzene concentrations; and *(D)* estimated SA values calculated using the component flux method for sources chosen to provide best fit of benzene concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).

The dotted line in figure 9*A* shows benzene concentrations calculated by StreamVOC using modified benzene concentrations for ground-water sources and Horn Pond Brook to provide a best fit to the measured concentrations by minimizing χ^2 defined in equation 48 (see table 7). The optimization added benzene sources in zones 1, 2, 3, 5, 9, and 10 with concentrations of 0.012, 0.0084, 0.013, 0.0046, 0.030, and 0.038 µg/L, respectively, and increased the concentration of benzene in Horn Pond Brook from 0.050 to 0.054 µg/L (table 7). The sources in zones 9 and 10 were comparatively large to compensate for the aeration and concomitant VOC loss over the weir at the end of zone 9 and the increase in benzene measured between zones 9 and 10.

The SAs calculated by StreamVOC for the optimized sources are shown in figure 9*C*. Comparing the SA of the Horn Pond Brook source in figure 9*B* with the corresponding SA results in figure 9*C* shows that α_{HPB} decreased from about 90 percent to approximately 50 percent between the two source input data sets.

SAs for benzene calculated using the component flux method and the optimized sources are shown in figure 9*D*. Comparing figure 9*C* with figure 9*D* shows the difference between the net flux method and component flux method in the case of a VOC with a surface-water concentration that is supersaturated with respect to Henry's Gas Law equilibrium yet with a relatively high atmospheric concentration (for example, benzene almost reaches Henry's Gas Law equilibrium in zones 5, 6, and 7). In the net flux method, there is no change in any of the α values in the absence of sources or at the dam and weir. In contrast, in the component flux method $\alpha_{BEN,AIR}$ increases if no other sources are influencing benzene. Furthermore, large step increases in $\alpha_{BEN,AIR}$ are seen at the dam and weir because benzene has a relatively low Henry's Gas Law solubility and the hydraulic structures are very efficient at promoting exchange for an insoluble gas. The net effect on the SA calculations is that at the downstream end of zone 10, the component flux method results in $\alpha_{BEN,AIR} = 20$ percent. In contrast, the net flux method yields $\alpha_{BEN,AIR} = 0$ at the same location.

Methyl *tert*-Butyl Ether

The synoptic sampling effort identified four sources of MTBE for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1, ground-water sources entering zones 1 and 9, and Horn Pond Brook. The synoptic-based inputs lead to model-simulated MTBE concentrations (shown as the solid line in fig. 10*A*) that are in reasonable agreement with the measured concentration values (data points). As an example, the synoptic-based inputs simulate the existence of an increase in MTBE concentration downstream from the confluence between the Aberjona River and Horn Pond Brook, and a decrease in MTBE concentration from zone 8c to zone 9 due to the aeration of the stream at the dam. Both of these effects are seen in the model results in figure 10*A*. However, the measured increase of MTBE in zone 9 is not seen

in the model results using the MTBE inputs derived from the source synoptic study.

The dashed line (fig. 10*A*) was obtained after adjusting the MTBE sources to minimize χ^2 defined in equation 48. The optimization added sources in zones 2, 3, 5, 8c, and 10 with MTBE values of 0.078, 0.47, 0.71, 13.4, and 0.73 µg/L, respectively, increased MTBE for the sources already present in zones 1 and 9 to 0.92 and 16.7 µg/L, respectively, and decreased MTBE in Horn Pond Brook by approximately 20 percent to 3.23 µg/L (table 7). Using the modified sources, MTBE concentrations simulated by StreamVOC are in excellent agreement with MTBE concentrations measured during the source synoptic study. Interestingly, nearly the same modifications required for MTBE also were required in the case of benzene. In particular, it was necessary to add relatively large sources for both MTBE and benzene in zone 5 and zone 9.

SA results corresponding to the synoptic-based inputs are given in figure 10*B*; SA results corresponding to the modified inputs are given in figure 10*C*. For the synoptic-based simulation, approximately 86 percent of the MTBE in the water is from Horn Pond Brook at the end of zone 10 (fig. 10*B*). In contrast, for the optimized sources, only 34 percent of the MTBE is from Horn Pond Brook (fig. 10*C*), with the difference in $\alpha_{MTBE,HPB}$ between the two cases due mainly to the effect of the source in zone 9 for the optimized case.

The SA results for MTBE using the optimized sources and the component flux method are shown in figure 10*D*. Although $\alpha_{MTBE,AIR}$ is greater than zero, there is little difference between the net flux method and component flux method for MTBE. This is because the MTBE concentration is substantially greater than Henry's Gas Law equilibrium over much of the source synoptic study region and its relatively high solubility decreases the effectiveness of the hydraulic structures on the exchange of MTBE between water and air.

Chloroform

The synoptic sampling effort identified three sources of chloroform for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1 and ground water entering zones 3 and 10.

The model-simulated concentrations (solid line in fig. 11*A*) based on the inputs from the synoptic sampling, however, do not lead to a good match with the measured concentrations. In particular, the synoptic-based inputs result in a concentration peak extending over zones 3 through 7 that is not observed in the measured concentrations. One possible reason is that the ground-water concentration of 1.16 µg/L greatly overestimates the true average chloroform concentration in the zone 3 ground-water source.

The dotted line in figure 11*A* shows model-simulated chloroform concentrations using modified concentrations for ground-water sources and Horn Pond Brook to give the best overall fit to the measured concentrations (table 7). The changes to the source concentrations that were required to minimize χ^2 were as follows: ground-water sources were added in
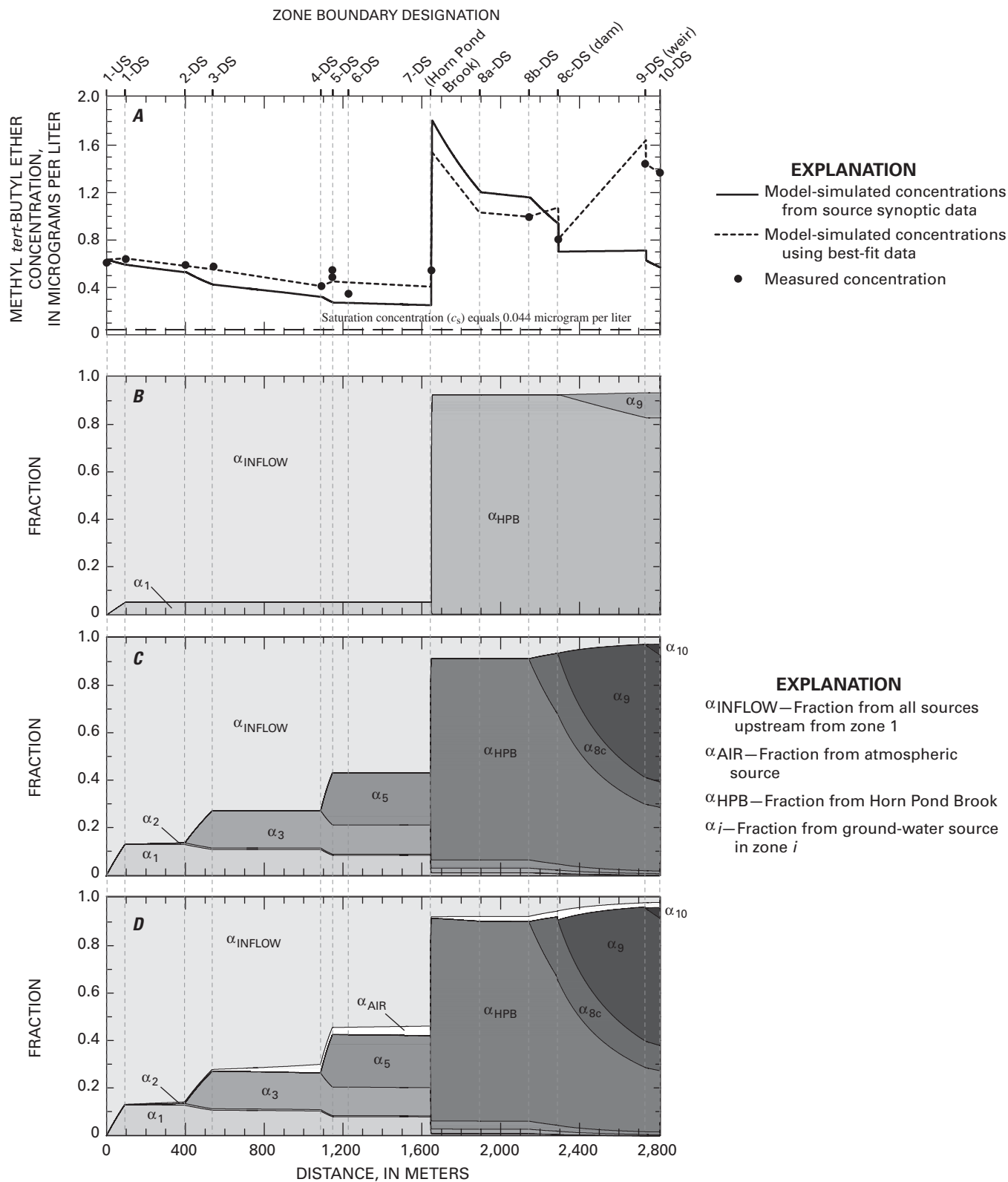
Figure 10. Methyl *tert*-butyl ether (MTBE) in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; *(C)* estimated SA values for sources chosen to provide best fit of MTBE concentrations; and *(D)* estimated SA values calculated using the component flux method for sources chosen to provide best fit of MTBE concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).

zones 1, 2, 5, 8c, and 9 with concentrations of 0.19, 0.20, 0.26, 2.82, and 0.56 µg/L, respectively; a chloroform source from Horn Pond Brook was added by increasing chloroform in Horn Pond Brook from 0 to 0.16 µg/L; the chloroform was decreased for the source in zone 3 from 1.16 to 0.19 µg/L; and the source in zone 10 was eliminated. The corresponding modified SA results for these new inputs are given in figure 11*C*. The SA calculations for the synoptic data set shown in figure 11*B* show that 25 percent of the chloroform at the end of the study region came from the ground-water source in zone 3, with 65 percent coming from the source in zone 10. In contrast, the SA calculations for the modified sources show that less than 5 percent of the chloroform in the water at the end of zone 10 is from zone 3, with the largest source fractions now due to sources in zones 8c and 9.

The solubility of chloroform is similar to that of benzene; therefore, chloroform and benzene are affected in a similar manner by the dam spillway and weir at the ends of zones 8c and 9, respectively. Relatively large sources are required in zones 8c and 9 to balance the simulated loss in VOC concentrations by aeration at the structures. As described in the following sections, this is a common feature of the model results for the chlorinated VOCs modeled in this study, all of which were outgassing from the stream.

The SA results for the component flux method using the optimized source inputs are shown in figure 11*D*. The atmospheric concentration of chloroform is small so that the stream is outgassing and never close to equilibrium in the synoptic study region. Therefore, $\alpha_{CLF,AIR}$ is only a few percent at the downstream end of zone 10.

1,1-Dichloroethane

The synoptic sampling effort identified three sources of 1,1-DCA for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1 and ground water entering both zones 1 and 5. The inputs from the synoptic sampling lead to model results (solid line in fig. 12*A*) that qualitatively capture some of the changes observed in the measured concentrations. For example, the concentration increase occurring within zones 4 and 5, the decrease that occurs over zone 3 due to the VOC flux to the atmosphere and dilution from ground-water inflow, and the decrease that occurs in zone 8a because of dilution from Horn Pond Brook. The synoptic-based inputs, however, do not lead to a good quantitative match between the model-simulated results and the measured concentration data. In particular, the input from ground water over zone 1 leads to an overestimation of 1,1-DCA concentrations from zones 2 to 4, and the input from ground water over zone 5 leads to an underestimation of the concentrations from zones 5 to 10. The SA calculations for the synoptic study sources shown in figure 12*B* indicate that at the end of zone 10, the three synoptic study-based sources each have an SA fraction of approximately one-third.

The dotted line in figure 12*A* shows model-simulated concentrations obtained after modifying the model input ground-water concentrations to minimize χ^2 defined in equation 48. The results were that the 1,1-DCA ground-water concentration was reduced in zone 1 from 0.48 to 0.0033 µg/L, the concentration was increased in zone 5 from 0.12 to 0.55 µg/L, ground-water 1,1-DCA sources were added in zones 2, 3, 8c, and 9 with concentrations of 0.26, 0.047, 1.15, and 0.36 µg/L, respectively, and the concentration in Horn Pond Brook was increased from 0 to 0.13 µg/L (table 7). Corresponding SA results for the modified sources are given in figure 12*C* and indicate that there is no dominant source of 1,1-DCA in the water at the end of zone 10. Similar to benzene, chloroform, and MTBE, relatively large sources were required in zones 8c and 9 to offset the loss of 1,1-DCA through aeration at the dam and weir. Because the atmospheric concentration of 1,1-DCA was zero, there is no difference between the net flux method and component flux method.

cis-1,2-Dichloroethene

The synoptic sampling effort identified five sources of *cis*-1,2-DCE for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1, ground water entering zones 1, 5, and 9, and the water entering from Horn Pond Brook. For zones 1 and 2, the synoptic-based inputs lead to model-simulated concentrations (solid line in fig. 13*A*) that agree with the measured concentrations. Also, for zones 5 through 8c, there is a general downward concentration trend both in the model results and in the measured data, including the marked drop in concentration caused by the dilution from the inflow of Horn Pond Brook at the beginning of zone 8a. However, for zones 5 through 10, the model-simulated concentrations are a factor of two less than the measured concentrations.

The SA calculations for the *cis*-1,2-DCE inputs identified in the synoptic study are shown in figure 13*B*. In this case, the two major sources of *cis*-1,2-DCE at the end of zone 10 are the source due to the water entering the study region at the beginning of zone 1 and the ground-water source in zone 9.

The dashed simulation line (fig. 13*A*) was obtained after optimizing the *cis*-1,2-DCE inputs by minimizing χ^2 defined in equation 48. This process resulted in the addition of *cis*-1,2-DCE sources in zones 3 and 8c with concentrations of 0.54 and 3.59 µg/L, respectively; increasing *cis*-1,2-DCE for the sources in zones 5 and 9 and Horn Pond Brook to 0.68, 1.04, and 0.33 µg/L, respectively; and eliminating the ground-water source of *cis*-1,2-DCE in zone 1 (see table 7). The SA results for these optimized sources are shown in figure 13*C* and indicate that in this case there is no dominant source of *cis*-1,2-DCE to the Aberjona River in the study region.

As was the case with 1,1-DCA, the atmospheric concentration of *cis*-1,2-DCE was zero. Therefore, there is no difference in the SA results between the net flux method and component flux method.
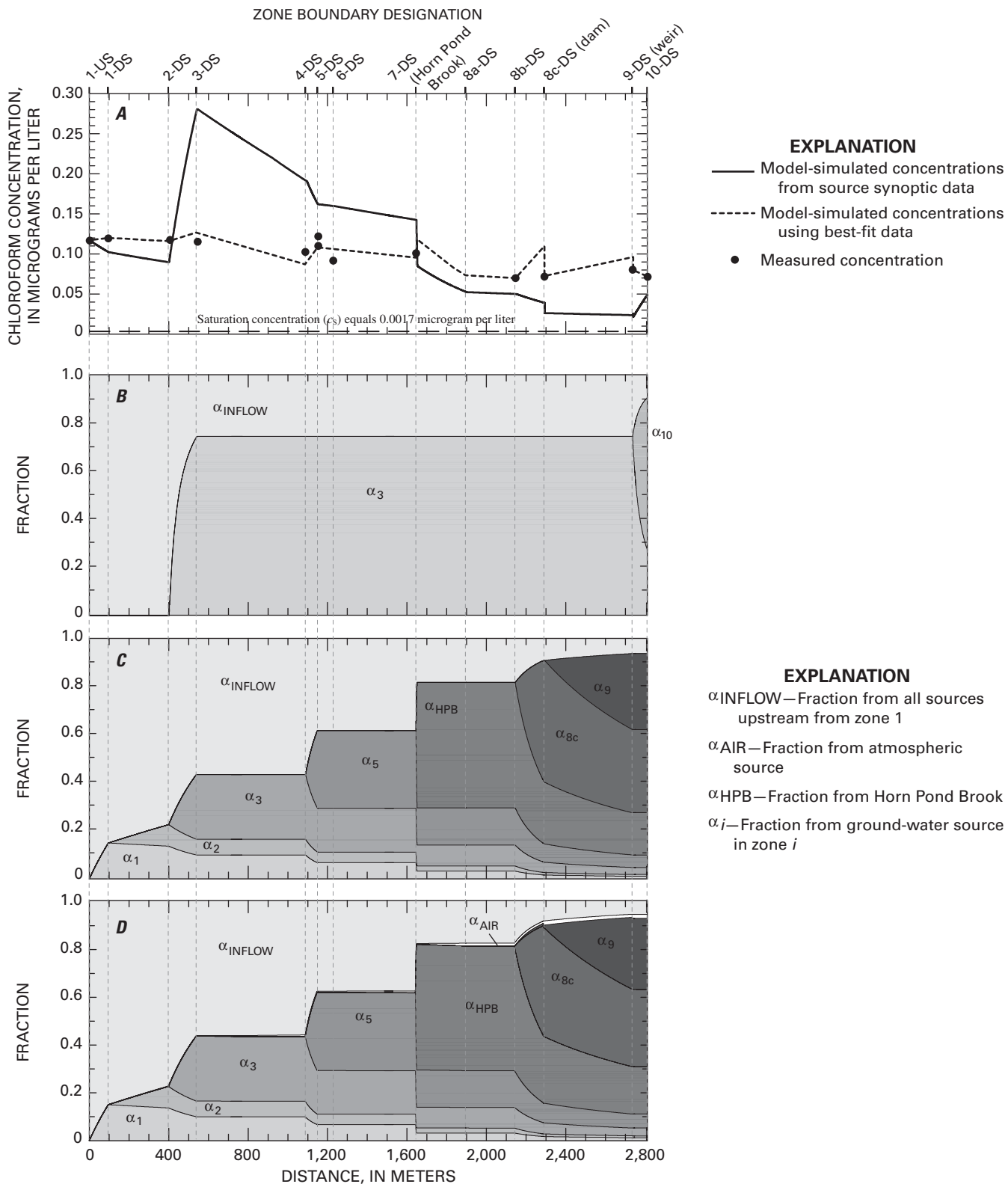
Figure 11. Chloroform in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; *(C)* estimated SA values for sources chosen to provide best fit of chloroform concentrations; and *(D)* estimated SA values calculated using the component flux method for sources chosen to provide best fit of chloroform concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).
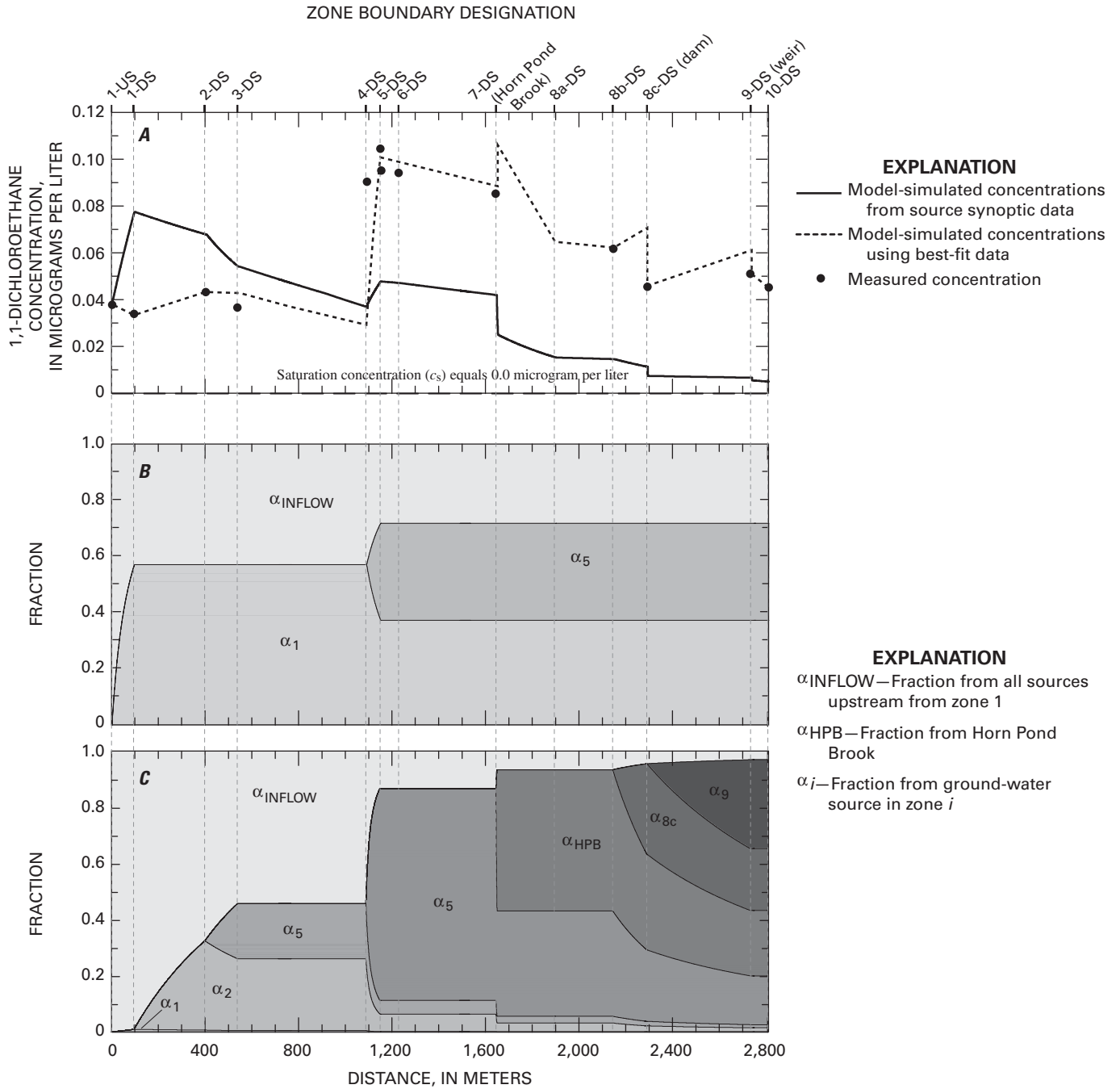
Figure 12. 1,1-Dichloroethane (1,1-DCA) in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; and *(C)* estimated SA values for sources chosen to provide best fit fo 1,1-DCA concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).
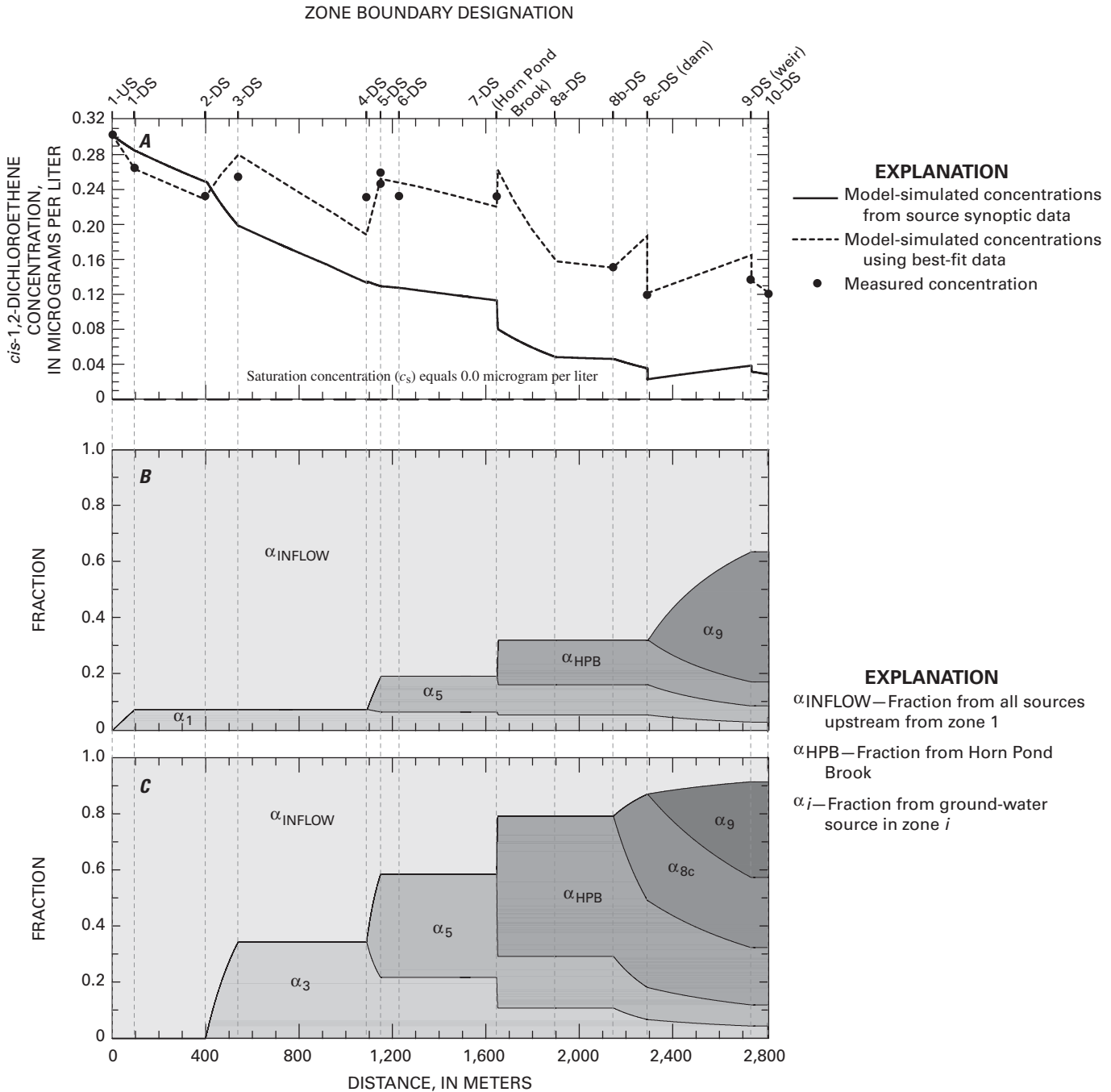
Figure 13. *cis*-1,2-Dichloroethene (*cis*-1,2-DCE) in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; and *(C)* estimated SA values for sources chosen to provide best fit of *cis*-1,2-DCE concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).

Trichloroethene

The synoptic sampling effort identified five sources of TCE for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1, ground water entering zones 1, 3, and 5, and the tributary flow from Horn Pond Brook. The synoptic-based inputs lead to model results (solid line in fig. 14*A*) that qualitatively capture the changes observed in the measured concentrations but underestimate the measured concentrations from zones 5 through 10. SA results corresponding to the synoptic-based simulation are given in figure 14*B*.

The dashed simulation line (fig. 14*A*) was obtained by optimizing the TCE sources to minimize χ^2 for TCE defined in equation 48. The optimization found the minimum χ^2 was obtained by decreasing TCE for the source in zone 3 from 0.39 to 0.26 µg/L, adding VOC sources in zones 2, 8c, 9, and 10 with concentrations of 0.14, 6.45, 0.65, and 0.19 µg/L, respectively, and increasing TCE in Horn Pond Brook and the TCE source in zone 5 to 0.34 and 1.65 µg/L, respectively (table 7). The corresponding SA results for the modified sources are given in figure 14*C*.

The SA results for the synoptic study sources show that the ground-water sources in zones 1, 3, and 5 account for nearly two-thirds of the TCE in the water at the end of zone 10. In contrast, the SA calculations for the modified sources indicate that only 18 percent of the TCE is due to ground-water inflow from these same zones. As observed for 1,1-DCA and *cis*-1,2-DCE, the downstream sources had a larger effect on TCE concentrations at the end of the synoptic study region than sources farther upstream. The SA results in figure 14*C* show that in the modified source cases, nearly one-half of the TCE in the Aberjona River at the downstream end of zone 10 is due to the sources in zones 8c, 9, and 10. In both cases, Horn Pond Brook contributes less than 10 percent of the TCE to the river at the end of the study region.

The solubility of TCE is relatively low, so there are large decreases in TCE at the end of zones 8c and 9 due to aeration by the dam and weir, respectively. This simulated decrease in TCE at these locations requires adding large TCE sources upstream from the structures to compensate for the loss of VOC. The SA calculations made using the component flux method show that because of the low atmospheric concentration of TCE, $\alpha_{TCE,AIR} = 0.09$ percent at the downstream end of zone 10 for the optimized TCE sources.

Perchloroethene

The synoptic sampling effort identified two sources of PCE for the Aberjona River study interval: the stream inflow to the study interval at the upstream end of zone 1 and ground water entering over zone 3. The synoptic-based inputs lead to model-simulated results (solid line in fig. 15*A*) that agree with the measured concentrations in that both show (1) an increase in PCE concentration over zone 1 to zone 3; and (2) a decrease in PCE concentration caused by the inflow of Horn Pond Brook

water. However, the simulated synoptic-source inputs fail to capture the increase in concentrations from zone 3 to zone 6 and from zone 8c to zone 9, and do not show any effect of the dam spillway at the downstream end of zone 8c and the weir at the downstream end of zone 9.

The dashed simulation line (fig. 15*A*) was obtained after modifying the model inputs to minimize χ^2 defined in equation 48 as shown in table 7 by decreasing PCE for the source in zone 3 from 0.82 to 0.21 µg/L; adding PCE sources in zones 1, 2, 5, 8c, 9, and 10 with concentrations of 0.14, 1.08, 0.64, 8.78, 1.53, and 0.11 µg/L, respectively; and adding a source from Horn Pond Brook by increasing its PCE from 0 to 0.091 µg/L. There is much better agreement between the measured and model-simulated concentrations for PCE.

SA results calculated using the net flux method for the sources derived from the synoptic survey are given in figure 15*B*. Not surprisingly, the major source of PCE to the Aberjona River over the synoptic study region is the ground-water source in zone 3. The corresponding SA results for the modified PCE sources using the net flux method are given in figure 15*C*. The sources in zones 8c and 9 account for approximately 80 percent of the PCE in the stream at the end of zone 10. Because of the low atmospheric concentration of PCE, there is essentially no difference between the SA results for the net flux method and the component flux method. For example, using the optimized PCE inputs, $\alpha_{PCE,AIR} = 0.30$ percent at the downstream end of zone 10.

Synopsis of StreamVOC Simulation Results

The values for χ_i^2 in table 6 show that benzene, MTBE, and TCE were the three compounds for which the synoptic-based sampling inputs led to the best general agreement between the StreamVOC-simulated concentrations and the measured concentrations and that acetone was by far the worst. It is not clear why the model fails to capture any of the major changes in the measured surface-water concentration of acetone. However, in the case of benzene and MTBE, the major source of VOC in the synoptic study region was Horn Pond Brook. Because this was a surface-water source, the concentration for each compound along with the flow volume added to the stream (and the resulting source term equal to the product of the concentration and the flow) was more easily characterized in terms of the total mass input to the Aberjona River. Therefore, it is not surprising that the accuracy of the model in terms of reproducing the measured concentrations is best for benzene and MTBE because there were no other major sources of either VOC in the study region. Conversely, Horn Pond Brook was not a major source of any of the other six VOCs simulated in this study.

A second similarity between benzene and MTBE is that both show an increase in concentration between the downstream end of zone 8c and the downstream end of zone 10. This increase in the measured surface-water concentrations indicates
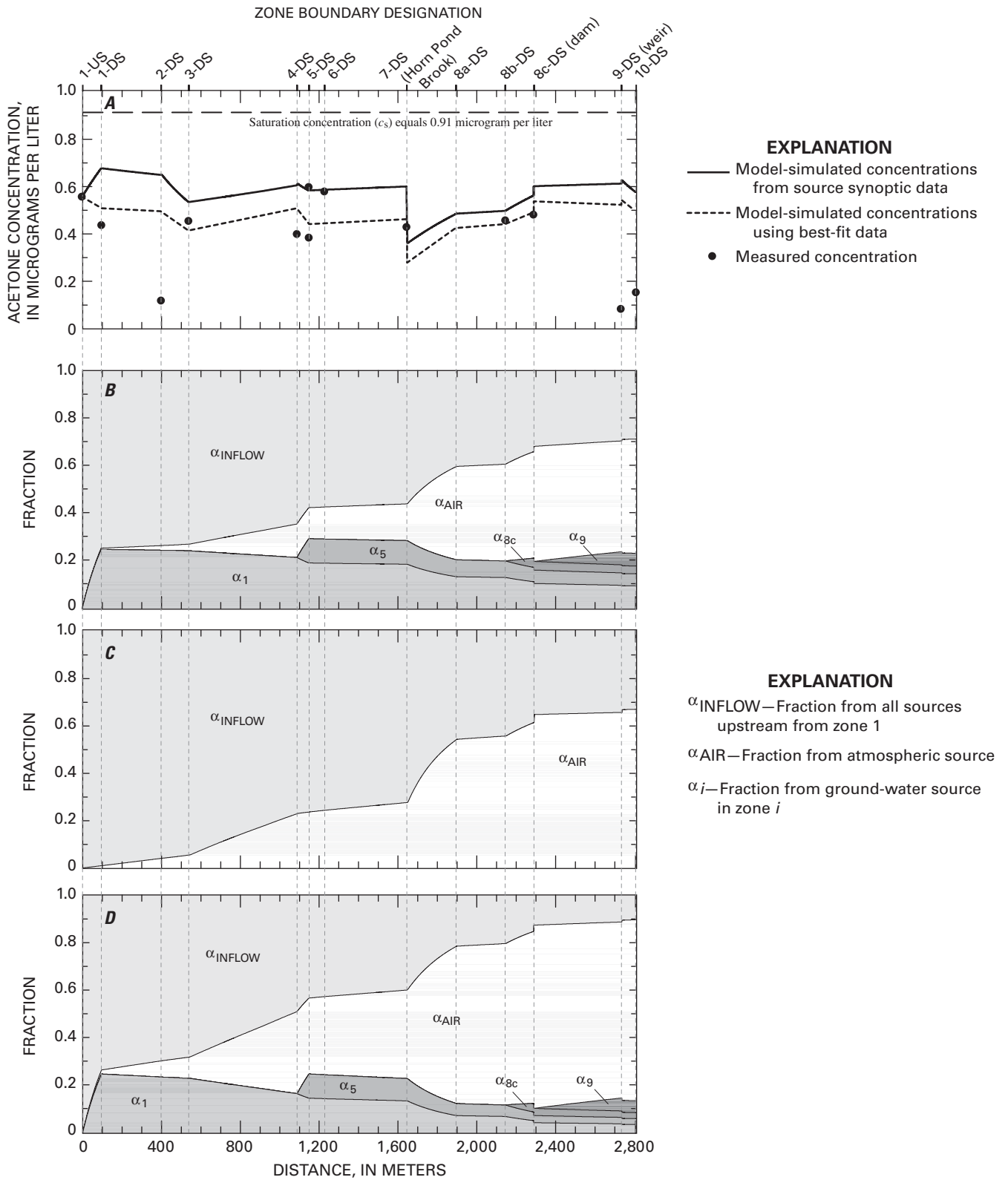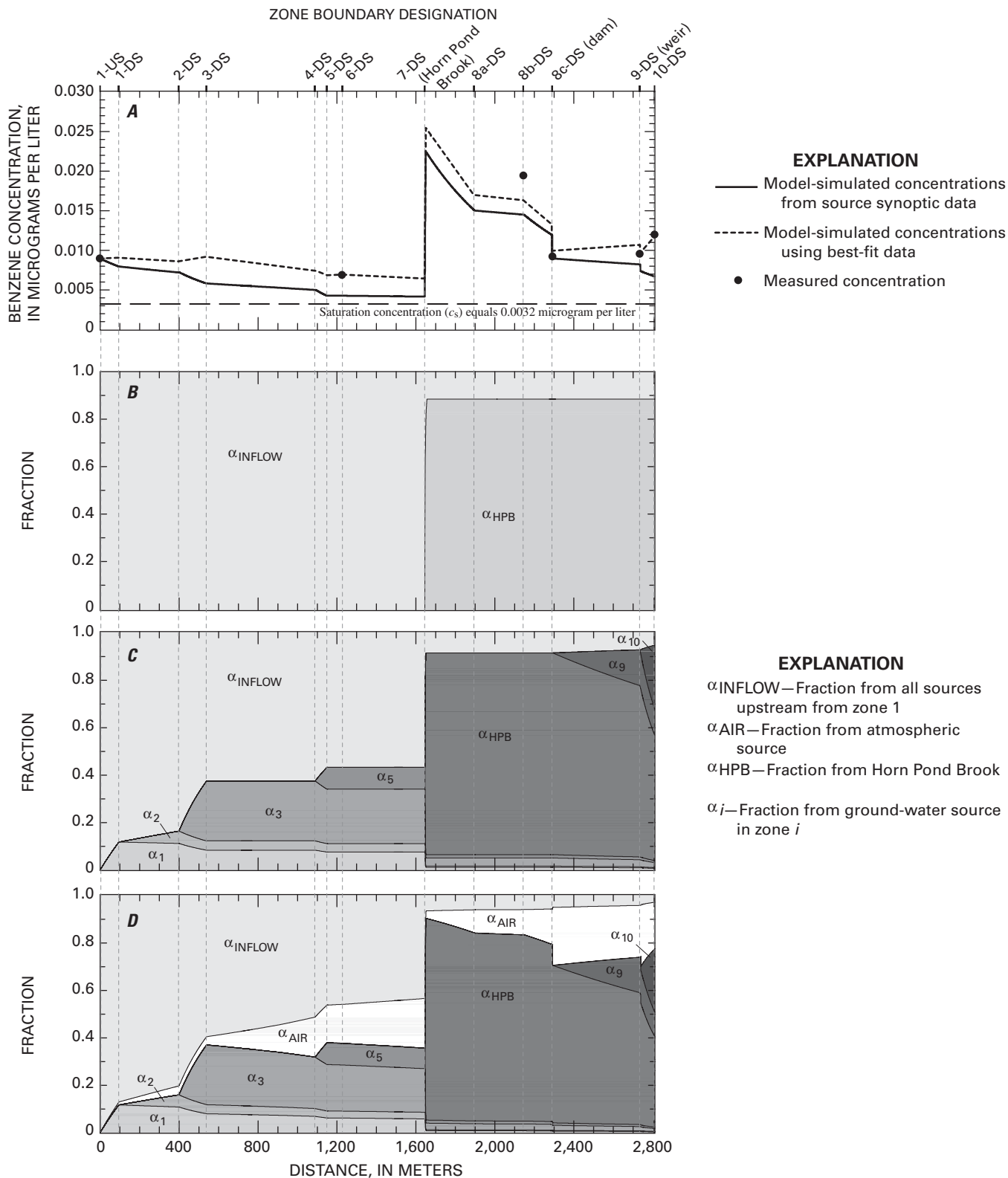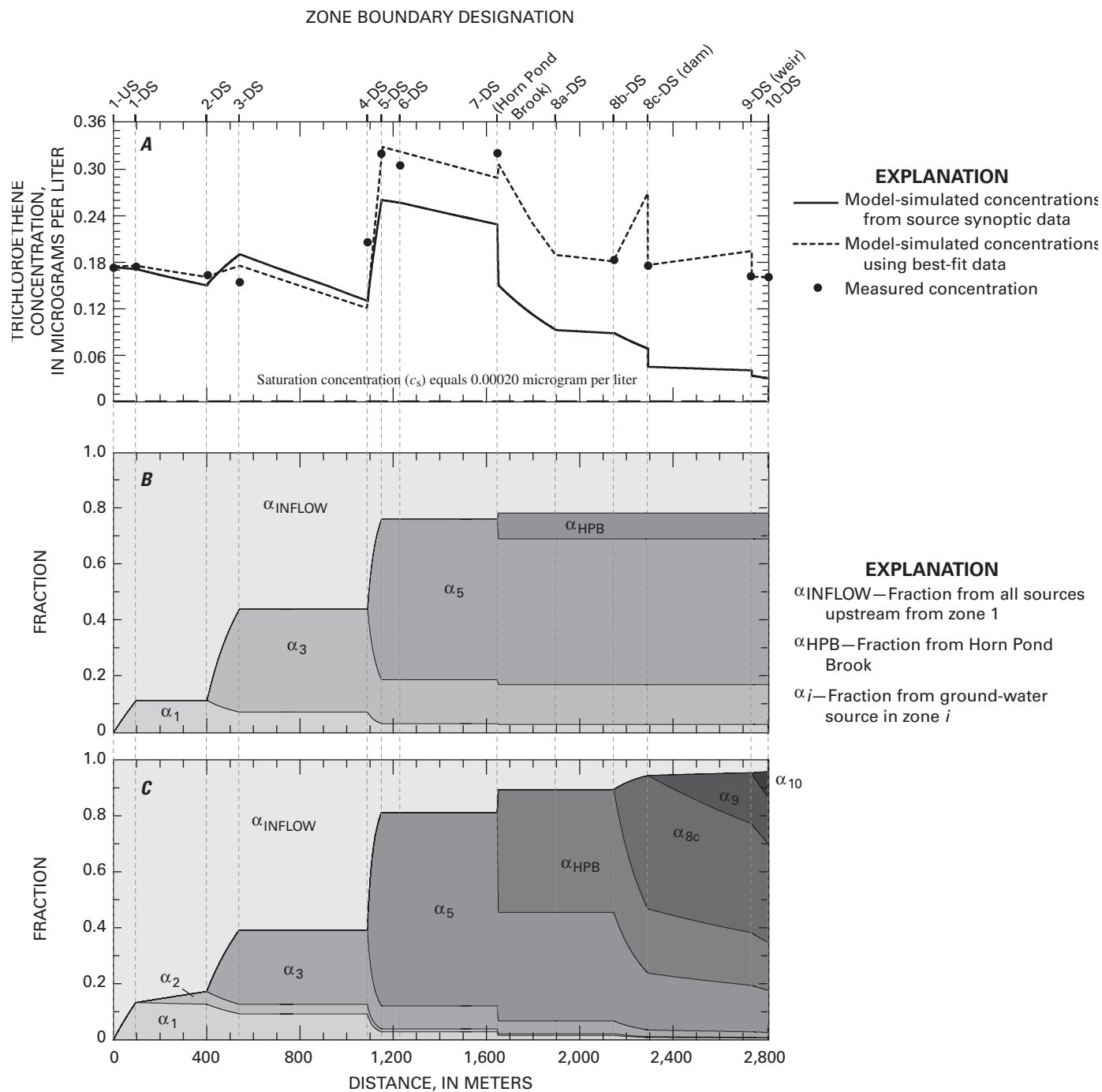
Figure 14. Trichloroethene (TCE) in the Aberjona River showing *(A)* concentrations; *(B)* estimated source apportionment (SA) values for sources derived from synoptic survey; and *(C)* estimated SA values for sources chosen to provide best fit of TCE concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).
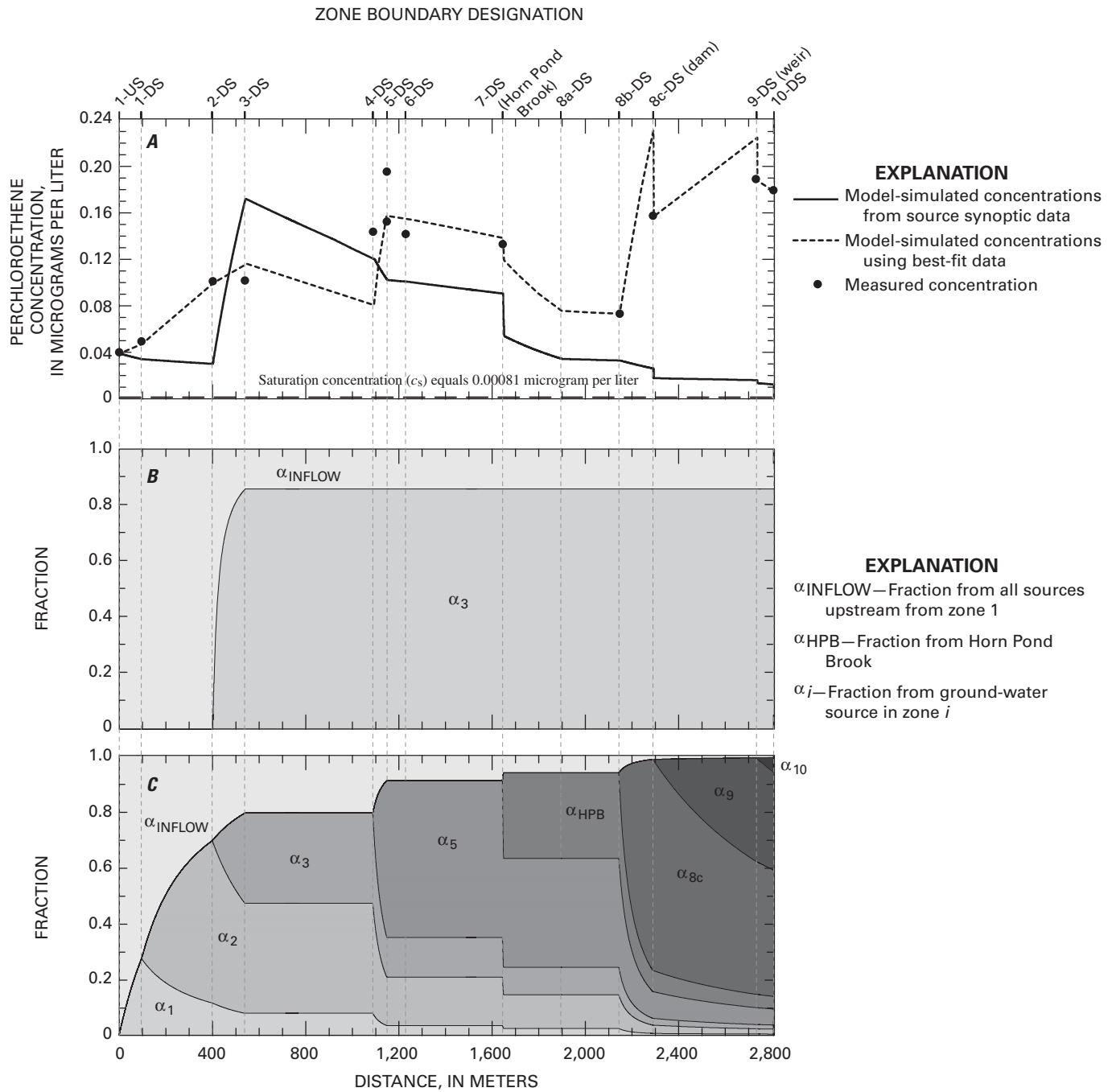
Figure 15. Perchloroethene (PCE) in the Aberjona River showing *(A)* concentrations; *(B)* estimated sources apportionment (SA) values for sources derived from synoptic survey; and *(C)* estimated SA values for sources chosen to provide best fit of PCE concentrations. Distance is measured going downstream (DS) from the upstream (US) end of zone 1 to the downstream end of zone 10 (see figure 6 for locations).

that there was a source for each VOC in those regions. Interestingly, in similarity with MTBE, the chlorinated compound PCE also shows a large increase in concentration in zones 9 and 10.

The major sources to the Aberjona River in the study area for the five chlorinated VOCs were due to ground-water inflows. Of these compounds, TCE yielded the best fit using the inputs derived from the synoptic data set. For 1,1-DCA and *cis*-1,2-DCE, the model results showed a similar trend between the simulated and the measured concentrations, although the absolute values of the simulated and measured concentrations differed on average by a factor of two for both compounds. For example, the synoptic-based inputs led to a decrease of about a factor of 2 in the simulated concentrations at the Aberjona/Horn Pond Brook confluence. Results for chloroform also showed a similar general trend between the simulated and measured concentrations, although it is evident that the simplistic estimate of $m_{in,i}(GW)$ for zone 3 was too large. For PCE, it is evident that the estimated inputs clearly fail to adequately characterize the sources to the Aberjona River. It is also clear that in the case of the chlorinated compounds, the model consistently underestimates the measured VOC concentrations in zones 4 through 10 when using the VOC inputs derived directly from the synoptic study data (note that because of the large chloroform source in zone 3, only zones 8a through 10 are underestimated for that VOC). This indicates that there were missing source terms for these compounds in the synoptic study region.

The data in table 7 show the changes in VOC sources resulting from minimizing χ^2 defined in equation 48. The modified source data in table 7 can be used to look for commonalities in changes to VOC sources required to simulate their concentrations in the Aberjona River. Figure 16 shows the difference between the VOC source concentration yielding the best fit to the measured and source VOC concentrations derived from the synoptic data set normalized by the average concentration of that VOC, β_i, plotted for each zone in the Aberjona River (note that zone 3b is not shown because it was not assumed to be a source or sink of VOCs). In order to plot differences on a common scale, they have been normalized by the average VOC concentration over the synoptic study region as:

$$\beta_i = \frac{\Delta[\text{VOC}]_i}{[\text{VOC}]_{i,\text{AVG}}}, \tag{49}$$

where $\Delta[\text{VOC}]_i$ is the difference between the modified source concentration and the best match source concentration determined from the synoptic study data set, and $[\text{VOC}]_{i,\text{AVG}}$ is the average concentration of the VOC over the synoptic study zone.

For the sources in zones 1 through 7, the results in figure 16 show that one modification required for all of the VOCs modeled here except acetone was an increase in the strength of the VOC source in zone 5. This indicates that the synoptic study measurements did not identify a source of VOCs to the Aberjona River in this area. In addition to the missing source in zone 5, there also is some evidence that an additional source is required in zone 2 in the case of benzene, MTBE, chloroform, 1,1-DCA, TCE, and PCE. Finally, the optimization

increased the concentrations of benzene, chloroform, 1,1-DCA, *cis*-1,2-DCE, TCE, and PCE in Horn Pond Brook. These increases are consistent with the observation that the sources derived directly from the synoptic study data led to the model consistently underestimating VOC concentrations in the latter zones in the region.

The other common modifications required were in the synoptic study zones downstream from the confluence of the Aberjona River with Horn Pond Brook. These modifications required adding a large VOC source in zone 9 for the seven VOCs that were outgassing to reconcile the simulated loss of VOCs due to aeration at the weir. Similarly, MTBE, chloroform, 1,1-DCA, *cis*-1,2-DCE, TCE, and PCE required a large source in zone 8c to compensate for the VOC loss at the dam spillway.

Flow under the dam and weir and the subsequent mixing as discussed previously could explain why the large decreases in VOC concentrations estimated by the optimization process using StreamVOC were not observed in measured concentrations. Assuming a value of κ typical for gravel (for example, $\kappa = 0.01$ m/s) gave what could be considered as the largest reasonable estimate for F_{under}. Using this, the two structures on the Aberjona River in the synoptic study region were characterized by values of F_{under} of approximately 20 percent. This value for F_{under} was used in StreamVOC, and χ_i^2 defined in equation 48 was minimized to incorporate the effects of flow under the weir on the surface-water concentrations and inferred source strengths.

Figure 17 shows the fractional change in the concentration of the VOC sources in Horn Pond Brook and zones 8c, 9, and 10, $\rho_{i,j}$, defined as

$$\rho_{i,j} = \frac{c_{i,j}(\text{no flow}) - c_{i,j}(\text{flow})}{c_{i,j}(\text{no flow})}, \tag{50}$$

where $c_{i,j}$ (no flow) is the optimized concentration of VOC i in source j assuming $F_{under} = 0$; and $c_{i,j}(\text{flow})$ is the optimized concentration of VOC i in source j assuming Q_{under} was $0.2Q$. We have defined $\rho_{i,j} = 0$ for cases where $c_{i,j}(\text{no flow})$ and $c_{i,j}$ (flow) are both zero although in a strict sense $\rho_{i,j}$ is undefined. Acetone is not shown in figure 17 because there was no effect of including flow under the weir on the optimization. The $\rho_{i,j}$ values show that except in the case of MTBE, in general the effect of including flow under the weir and dam is to decrease the concentration of $c_{i,j}$ in zones 8c and 9 by a factor of 0.2 to 0.3. Furthermore, except in the case of MTBE, there is no effect of including flow under the weir on the source concentration of the VOCs in Horn Pond Brook and zone 10. It is not clear why the $c_{MTBE,j}$ (flow) are so different from $c_{MTBE,j}$ (no flow). Figure 18*A* shows $c_{MTBE,j}$ (flow) and $c_{MTBE,j}$ (no flow), and for comparison figure 18*B* shows $c_{TCE,j}$ (flow) and $c_{TCE,j}$ (no flow), with the latter displaying the typical behavior of the other VOCs. Regardless of the details, the graphs of the concentrations show that for the VOCs included in the test model there is little effect of the flow under hydraulic structures on the downstream VOC concentrations.
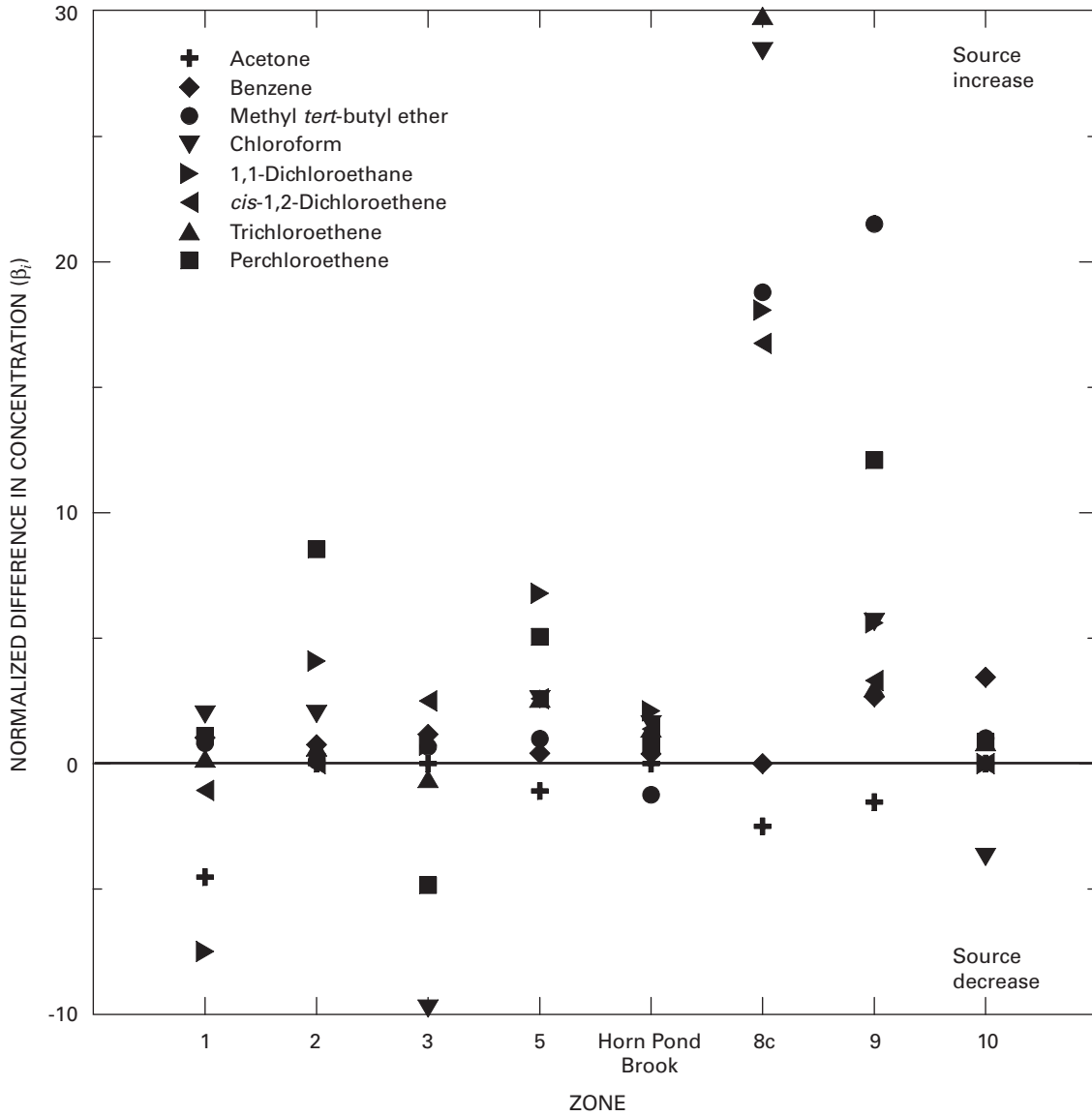
Figure 16. The difference between the source volatile organic compound (VOC) concentration yielding the best fit to the measured VOC concentrations and the source VOC concentration derived from the synoptic data set normalized by the average concentration of that VOC, β_i, as defined in equation 49 as the difference between the modified source concentration and the source concentration determined from the synoptic study data set, $\Delta[VOC]_i$, divided by the average concentration of the VOC over the synoptic study zone, $[VOC]_{i,AVG}$, and plotted for each zone in the Aberjona River synoptic study region. Note that the zone positions on the x-axis are not drawn to scale and do not represent actual distances between the zones.
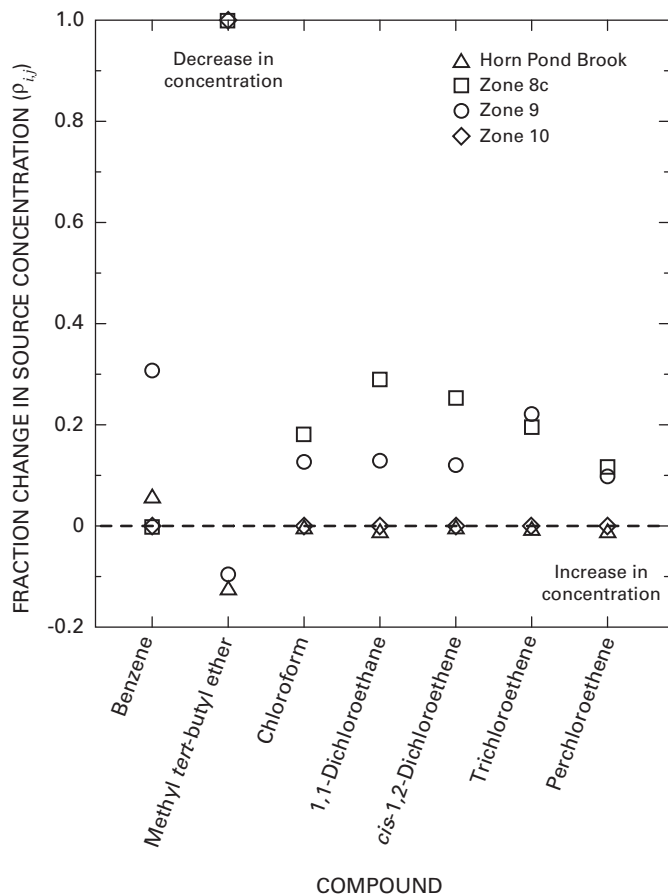
Figure 17. The fraction change in source concentration, $\rho_{i,j}$, caused by including the effect of flow of surface water under the dam at the downstream end of zone 8c and the weir at the downstream end of zone 9 for the volatile organic compound sources in Horn Pond Brook and zones 8c, 9, and 10. $\rho_{i,j}$ is defined in equation 50 as the difference between the optimized VOC concentration assuming no flow under the dam or weir, $c_{i,j}$ (no flow), and the optimized VOC concentration assuming that 20 percent of the total streamflow was under a hydraulic structure, $c_{i,j}$ (flow), divided by $c_{i,j}$ (no flow).

Therefore, it is unlikely that flow under structures is the cause of the large sources in zones 8c and 9 generated by the optimization.

Although the addition of large sources in these zones seems unrealistic, all available experimental and theoretical studies indicate that weirs and spillways have a large effect on dissolved gas concentrations (McLachlan and others, 1990; Gulliver and others, 1998; Urban and others, 2001; Caplow and others, 2004). Additionally, there is no evidence that indicates that gas fluxes were severely overestimated at the hydraulic structures (for example, the aeration efficiencies estimated by StreamVOC are correct insofar as they are being correctly calculated by the relations given previously). Finally, there is some experimental evidence supporting the existence of large sources in this region—the measured surface-water concentrations for

MTBE and PCE both show large increases over zones 8c and 9. But it also should be recognized that accurately estimating aeration at hydraulic structures from parameterizations such as used here is extremely difficult. Therefore, although there is no prior reason to assume that the VOC fluxes from the stream to the atmosphere due to the hydraulic structures are greatly overestimated by StreamVOC, the presence of large VOC sources in zones 8c and 9 is by no means certain based solely on the StreamVOC results.

VOC concentration measurements upstream and downstream from the weir and dam would provide evidence that the transfer efficiencies were being estimated correctly in the model. Because hydraulic structures can cause large changes in VOC concentrations, these additional concentration measurements also would help to parameterize VOC sources in a particular study region.

Sensitivity Analyses

Field measurements of the VOC concentrations, streamflows, stream widths, and stream depths that are the primary input data to StreamVOC are subject to uncertainties and measurement errors. Furthermore, the accuracy of the input data will affect the values calculated by the model. In order to assess this effect on the model output, a sensitivity study was conducted using the optimized source input concentrations, $c_{i,j}$, listed in table 7. The variation of the model-simulated surface-water concentrations was calculated for changes in $c_{i,j}$, h, w, and Q. The variation was calculated by running StreamVOC with the value of a variable in a zone increased by 10 percent, and a second simulation was run where the value was decreased by 10 percent. This was done on an individual basis so that in the case of h, for example, a total of 20 separate model runs were conducted. The maximum and minimum concentrations resulting from these calculations are shown in figures 19–26 for the eight VOCs included in the test model.

The results for the sensitivity analyses show that variations in source concentrations have the largest effect on the surface-water concentrations, followed by the source flows, with the effect of width and depth being relatively minor. Replicate samples are only available from the downstream end of zone 5. Furthermore, because only two replicates were collected, it is not possible to compute a standard deviation from the data at a single location. However, the point samples from the downstream ends of zones 4, 5, and 6 are all within 140 m of each other and combined they can be used to estimate concentration variances for each compound (except in the case of benzene, where only one concentration was measured to be above the MDL). The standard deviation is 24 percent of the mean for acetone, 20 percent for MTBE, 12 percent for chloroform, 8.5 percent for 1,1-DCA, 6.2 percent for *cis*-1,2-DCE, 18 percent for TCE, and 15 percent for PCE. By comparing the range of concentrations given by these standard deviations with the range of concentrations generated by StreamVOC based on the sensitivity test, it is seen that the sensitivity of the model is less than the

ZONE BOUNDARY DESIGNATION
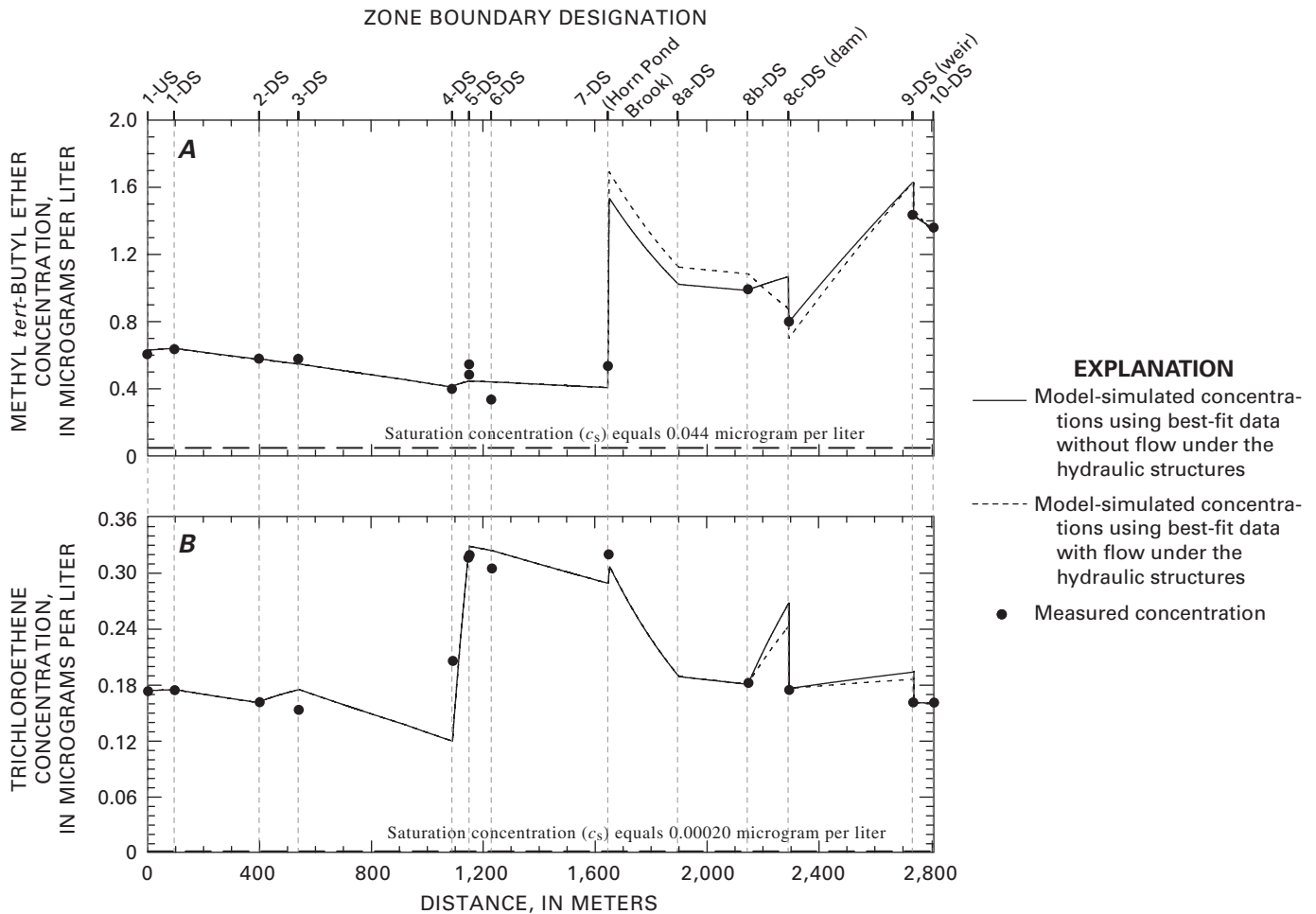
Figure 18. Model-simulated surface-water concentrations of *(A)* methyl *tert*-butyl ether for the condition where there is no flow of surface water under the hydraulic structures, c_{MTBE}(no flow), and when there is flow under the structure, c_{MTBE}(flow); and *(B)* trichloroethene assuming no flow under the weir and flow under the weir, c_{TCE}(no flow), and c_{TCE}(flow), respectively.

variance in the measured concentrations. This indicates that most of the larger changes in concentration as a function of sampling site observed in the surface-water synoptic study samples are not due solely to experimental noise and that the optimized source strengths could reflect the presence of sources not adequately accounted for using only the ground-water inflows determined from the synoptic study data set.

The assumption that the sources were distributed evenly over zones where the net streamflow increased is a simplification. It is understood that the distribution of sources in a zone could be a combination of small point sources and distributed sources that extend only over part of a zone. Although there is no best way to model a more complicated set of sources given the limitations of the source synoptic study data set, it is possible to determine whether the distribution of sources used here is a reasonable approximation to the true distribution of sources. Figure 27 shows the normalized difference between the measured and model-simulated concentrations (the modeled concentration was calculated using the optimized source inputs), $\gamma_{i,j}$, defined as

$$\gamma_{i,j} = \frac{[VOC]_{i,j,MEASURED} - [VOC]_{i,j,MODEL-SIMULATED}}{[VOC]_{i,AVG}} \quad (51)$$

plotted by zone number. In most cases, the values for $\gamma_{i,j}$ are scattered around zero, showing that there is no systematic pattern of overestimation or underestimation of the measured concentrations. However, there is some indication that the VOC concentrations at the downstream end of zone 4 were consistently underestimated, indicating the presence of a VOC source in the zone. Because zone 4 was a region where streamflow decreased, it was not possible to include a VOC source in this region using the assumption of continuous sources over an entire zone.

Model Limitations and Program Considerations

The results obtained in this study illustrate the great utility of SA concepts when seeking to (1) understand and identify the sources and sinks acting to determine location-dependent concentrations of contaminants in surface waters; and (2) determine potential courses of action for remediation and source
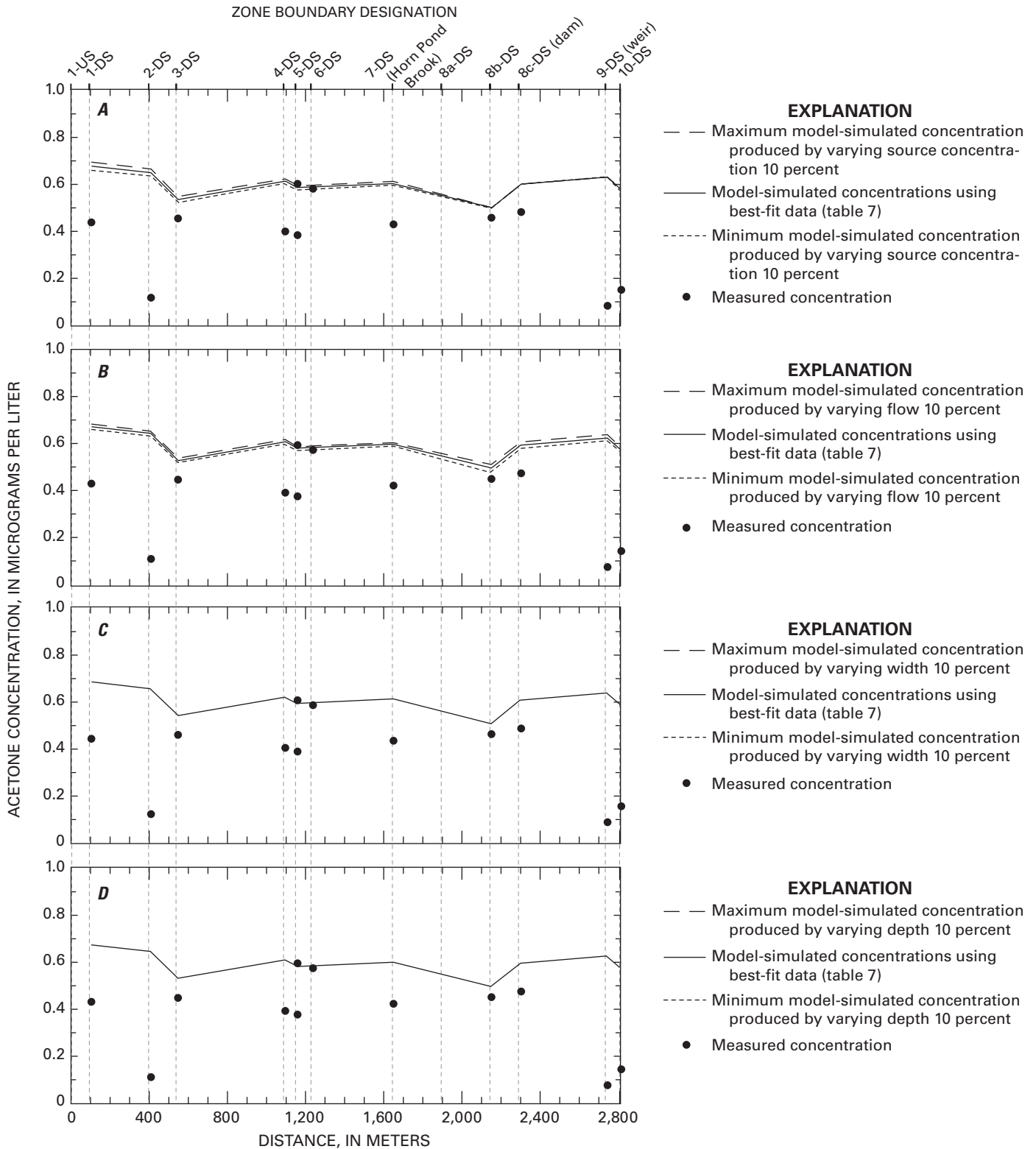
Figure 19. Results of model sensitivity analyses done for acetone using StreamVOC and the acetone sources determined from the source synoptic study data set by varying *(A)* the concentration of the individual acetone sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
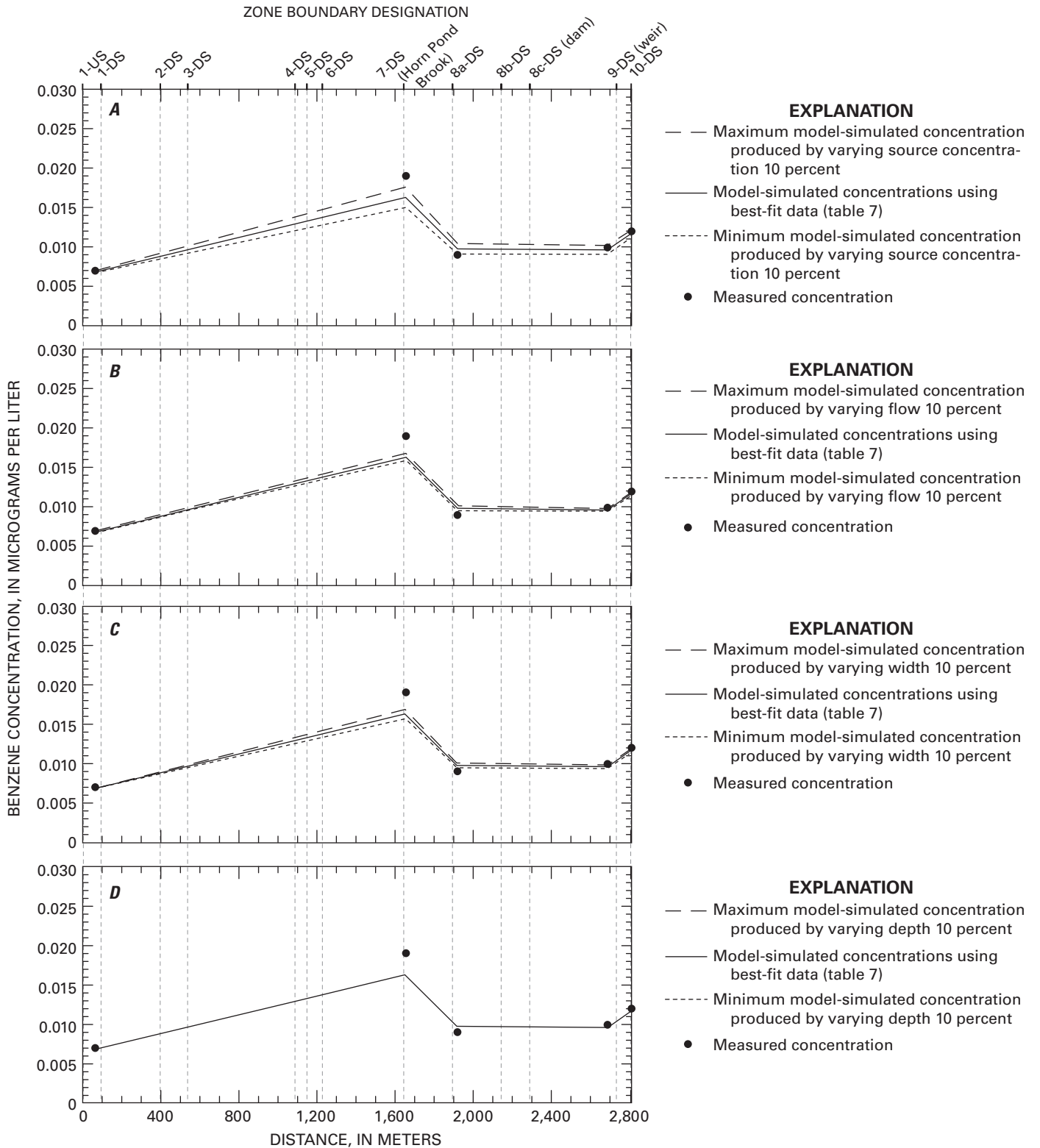
Figure 20. Results of model sensitivity analyses done for benzene using StreamVOC and the benzene sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual benzene sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
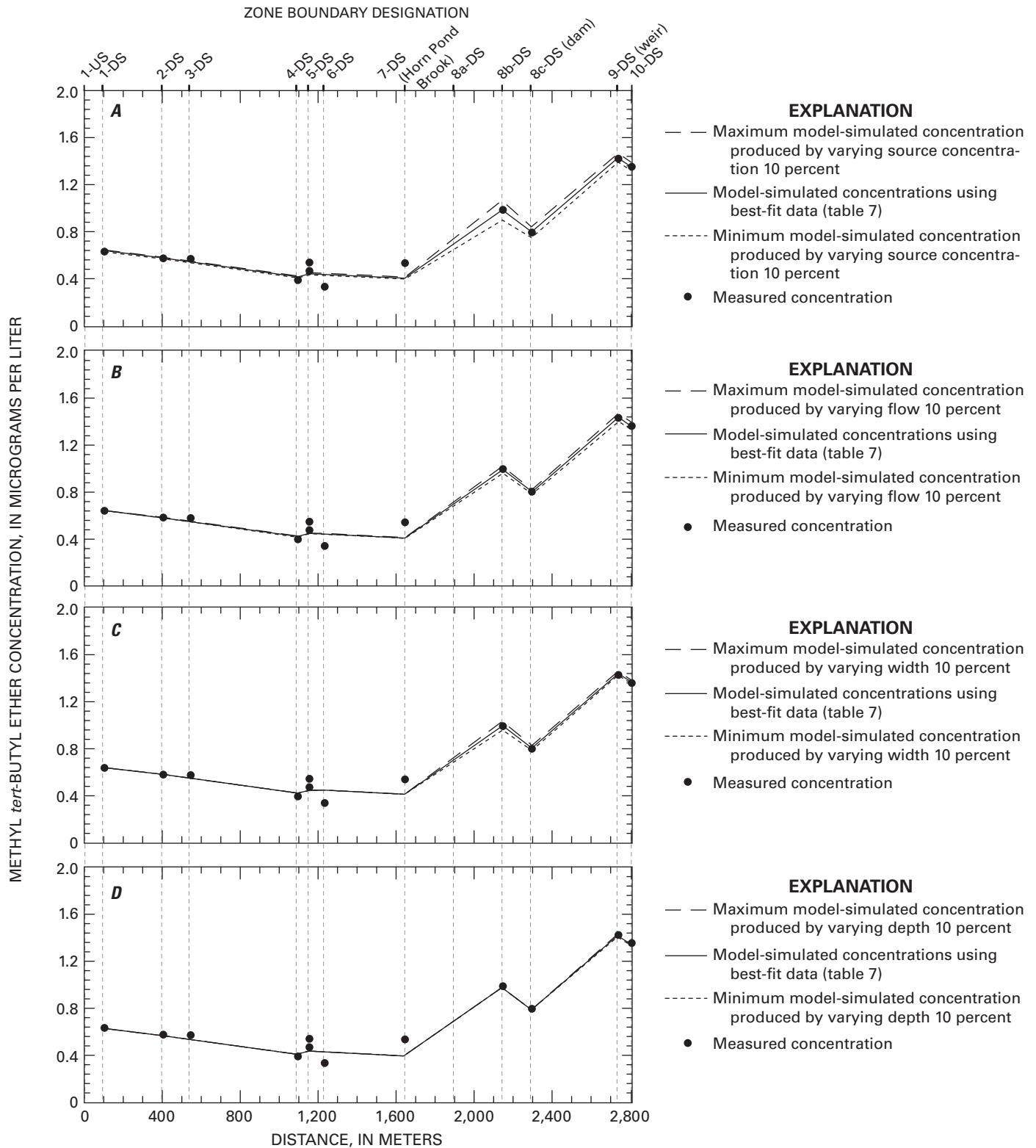
Figure 21. Results of model sensitivity analyses done for methyl *tert*-butyl ether (MTBE) using StreamVOC and the MTBE sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual MTBE sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
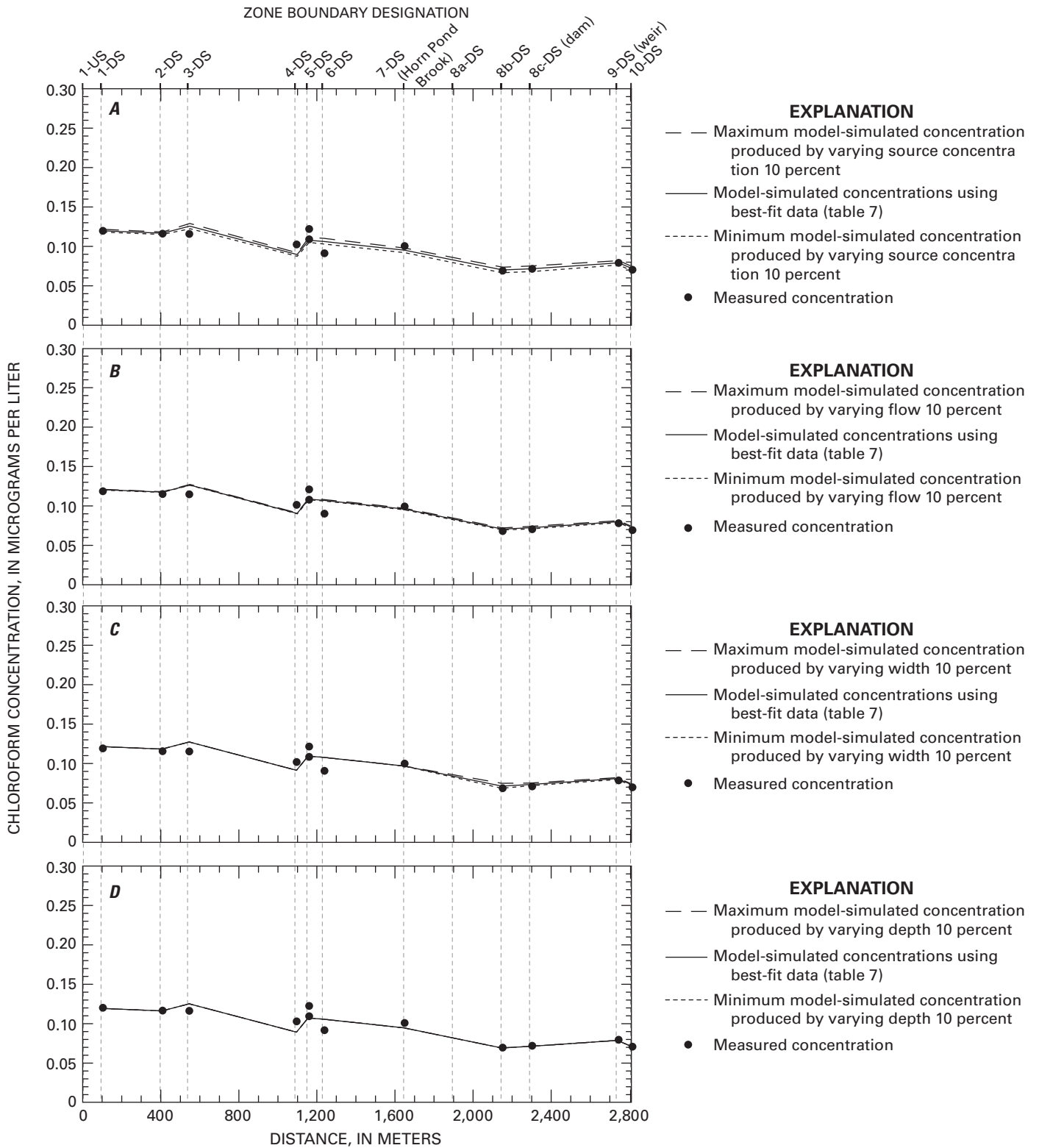
Figure 22. Results of model sensitivity analyses done for chloroform using StreamVOC and the chloroform sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual chloroform sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
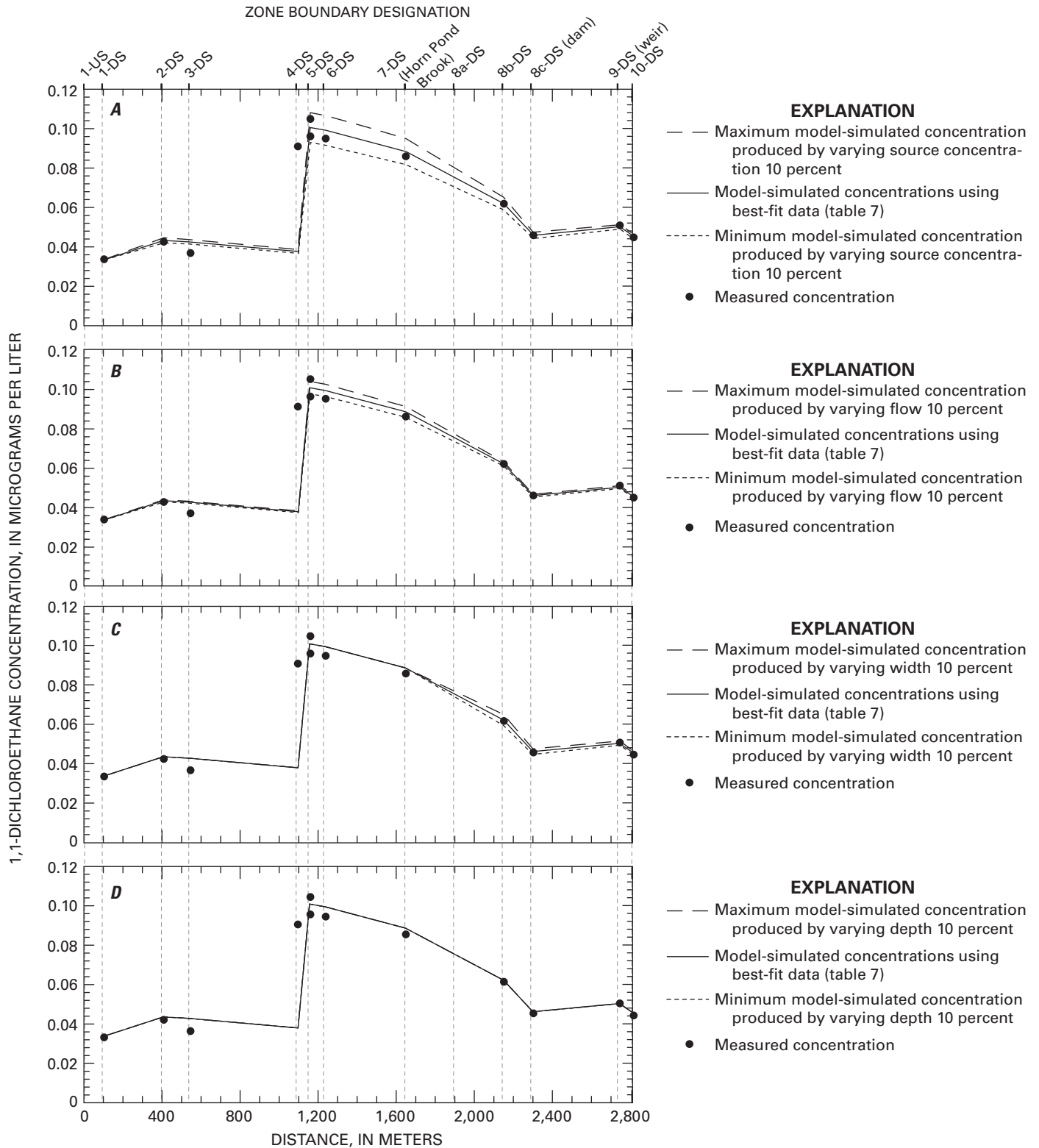
Figure 23. Results of model sensitivity analyses done for 1,1-dichloroethane (1,1-DCA) using StreamVOC and the 1,1-DCA sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual 1,1-DCA sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
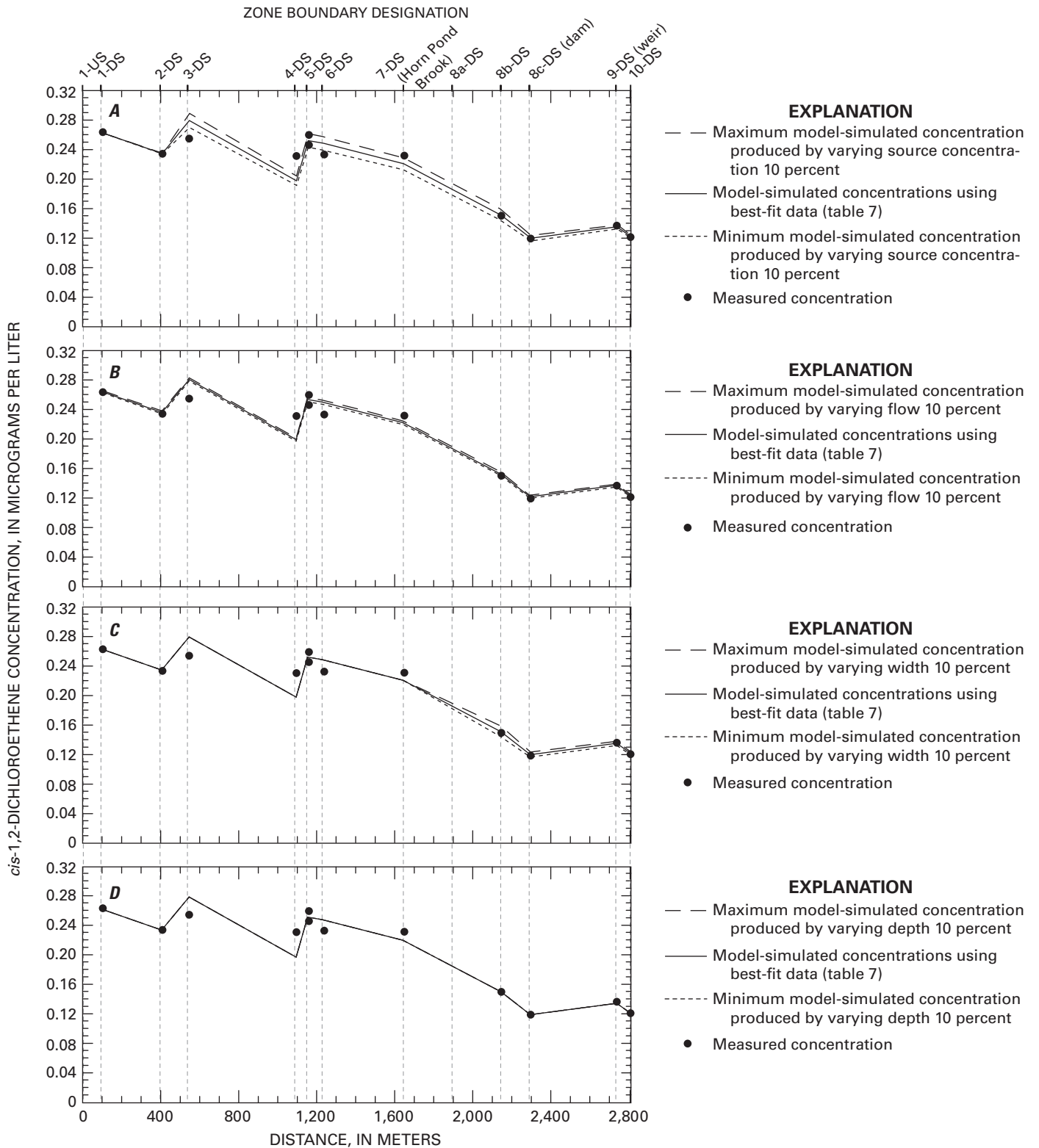
Figure 24. Results of model sensitivity analyses done for *cis*-1,2-dichloroethene (*cis*-1,2-DCE) using StreamVOC and the *cis*-1,2-DCE sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual *cis*-1,2-DCE sources; *(B)* the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
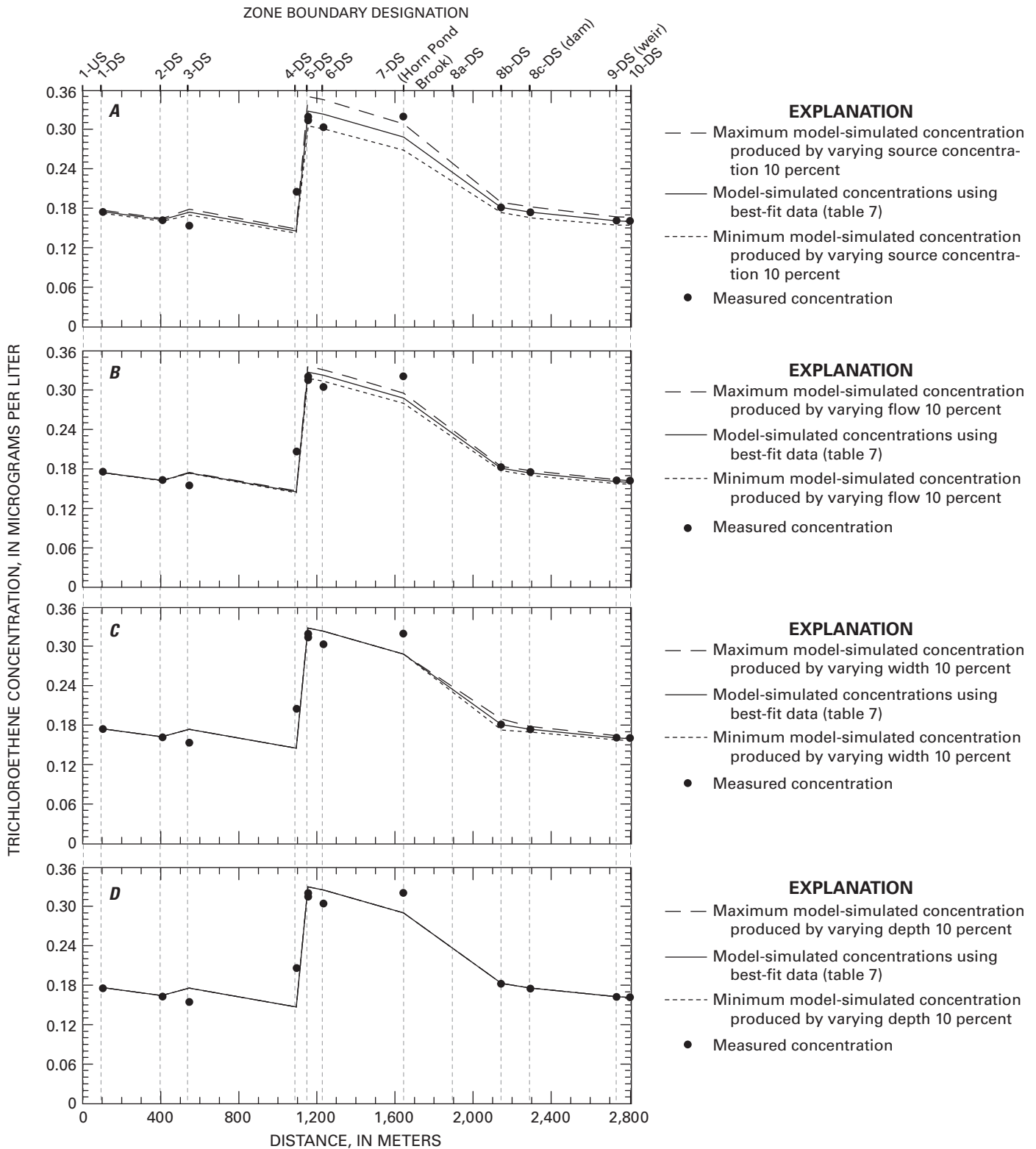
Figure 25. Results of model sensitivity analyses done for trichloroethene (TCE) using StreamVOC and the TCE sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual TCE sources; *(B)* the flow volumes of ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
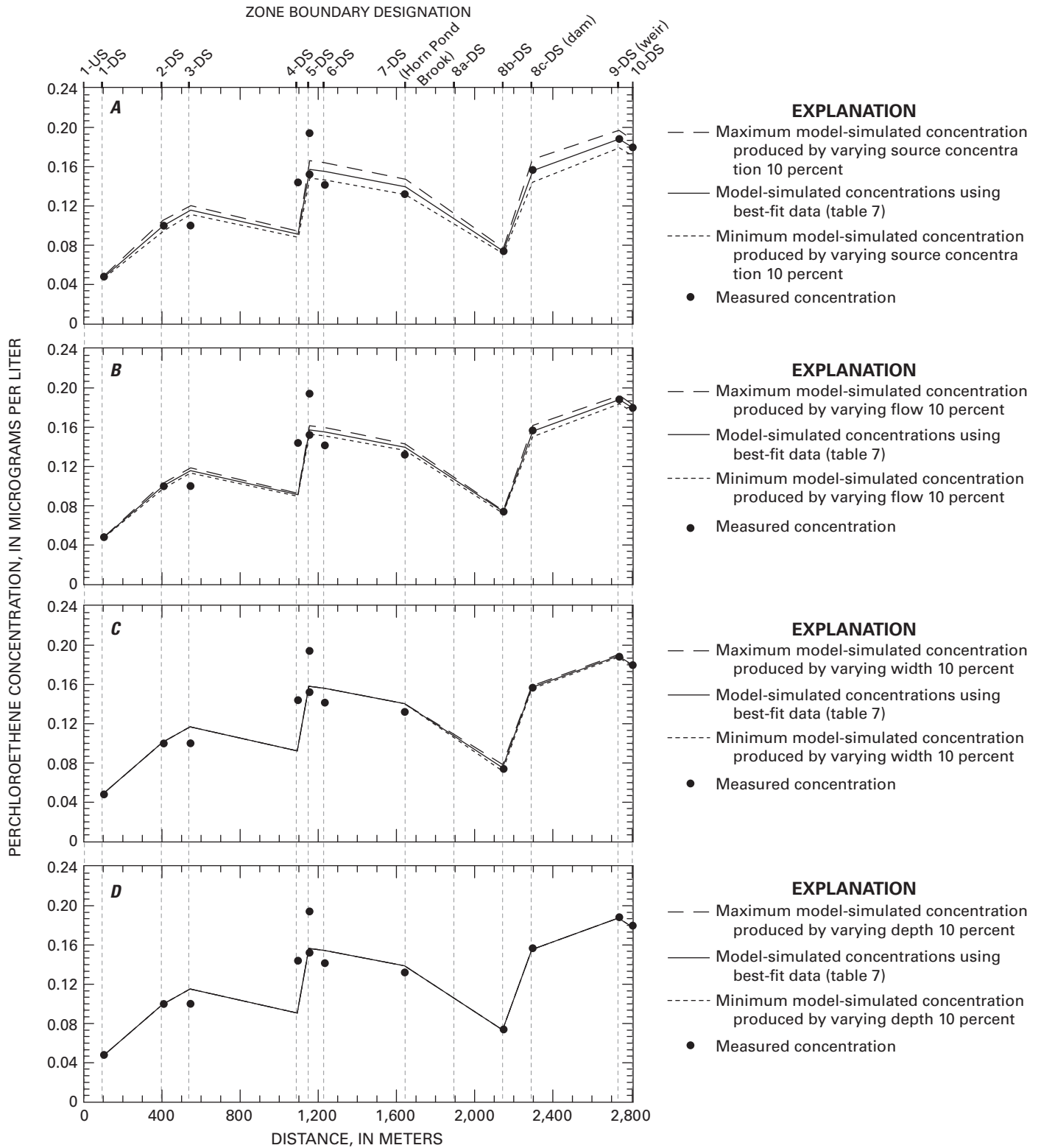
Figure 26. Results of model sensitivity analyses done for perchloroethene (PCE) using StreamVOC and the PCE sources determined by minimizing the reduced chi-square value between the measured surface-water concentrations and concentrations calculated using StreamVOC by varying *(A)* the concentration of the individual PCE sources; *(B)* in the flow volumes of the ground-water sources in each zone and in Horn Pond Brook; *(C)* stream width in each zone; and *(D)* stream depth in each zone.
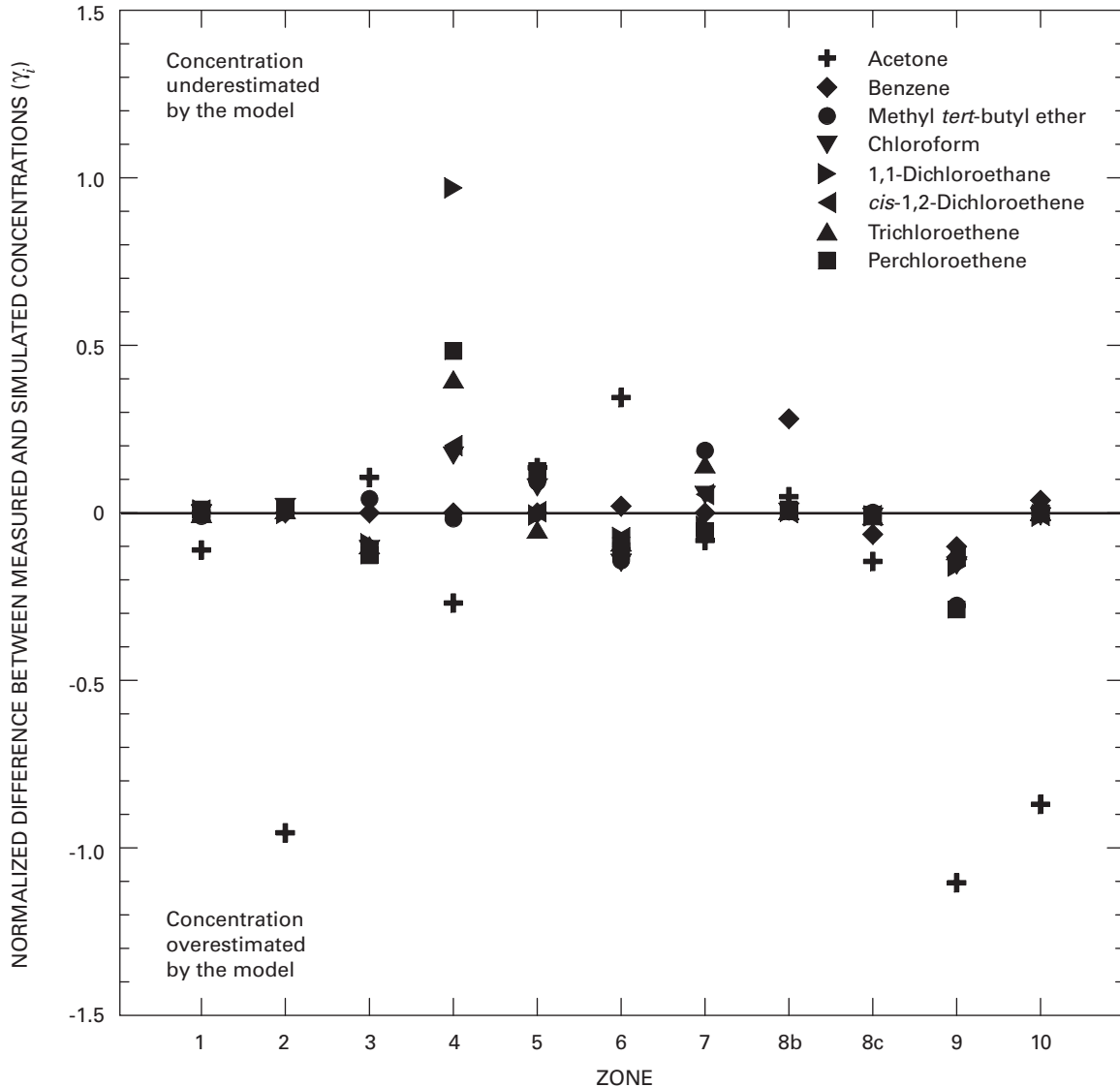
Figure 27. The normalized difference between the volatile organic compound (VOC) concentration measured in the Aberjona River and the VOC concentration simulated by the model using the optimized sources, $\gamma_{i,j}$, as defined in equation 51 as the difference between the measured and model-simulated concentrations divided by the average concentration over the synoptic study zone, and plotted for each zone in the Aberjona River source synoptic study region. Note that the zone positions on the x-axis are not drawn to scale and do not represent actual distances between the zones.

reduction in an effort to lower VOC concentrations in streams. For example, based on model results and subject to model limitations, reducing the MTBE and benzene contamination of Horn Pond Brook would be required in order to reduce the concentrations of these compounds in the downstream portion of the study section. As another example, for *cis*-1,2-DCE as simulated using the inputs determined from the synoptic data set, the source fractions show that at the downstream end of the study interval, more than 50 percent of the compound in the river is due to the initial inflow entering at the upstream end of zone 1. Thus, remediation of all *cis*-1,2-DCE sources along the

study interval could reduce the concentrations by, at most, a factor of two.

In general, this study illustrated (1) the considerable difficulty of quantifying correctly the locations and magnitudes of ground-water-related sources of contamination in streams; and (2) that model-based estimates of stream VOC concentrations are likely to be most accurate when the major sources are point sources or tributaries where the spatial extent and magnitude of the sources are tightly constrained and easily determined.

Summary

The National Water-Quality Assessment (NAWQA) Program of the U.S. Geological Survey seeks to understand the sources and processes that determine the concentrations, transport, and fate of contaminants in the natural waters of the United States. Contaminant groups of interest include volatile organic compounds (VOCs), and for urban streams, NAWQA results indicate the frequent presence of multiple dissolved VOCs. An adequate understanding, however, does not exist of the identities and relative roles of the typical contaminant sources that lead to the observed VOC concentrations, nor of the coupled manners in which physical, chemical, and biological processes in streams act on those contributions to yield observed position- and time-dependent concentrations. There is interest in the continued development of "source apportionment" (SA) modeling principles for use in tracking how multiple VOC sources and sinks can combine to yield a given observed concentration at some stream point (x, y, z, t). Reasons for interest in the relative and absolute contributions of different sources to VOC concentrations include the need to apportion: (1) the origins for observed contamination, and (2) the associated human and ecosystem risks.

This report documents the construction and verification of the model, StreamVOC, that estimates (1) the time- and position-dependent concentrations of volatile organic compounds (VOCs) in rivers and streams as well as (2) the source apportionment (SA) of those concentrations. The model considers how different types of sources and loss processes can act together to yield a given observed VOC concentration. For VOCs, sources of interest include the atmosphere (by absorption), as well as point and nonpoint inflows of VOC-containing water. Loss processes of interest include volatilization to the atmosphere, degradation, and outflows of VOC-containing water from the stream to local ground water.

This report presents the details of StreamVOC and compares model output with measured concentrations for eight VOCs—acetone, benzene, methyl *tert*-butyl ether (MTBE), chloroform, 1,1-dichloroethane, *cis*-1,2-dichloroethene (*cis*-1,2-DCE), trichloroethene, and perchloroethene—found in the Aberjona River at Winchester, Massachusetts. Input data for the model were obtained during a synoptic study of the stream system conducted July 11–13, 2001, as part of the NAWQA Program of the U.S. Geological Survey. The input data included a variety of basic stream characteristics (for example, flows, temperature, and VOC concentrations).

The StreamVOC concentration results agreed moderately well with the measured concentration data for several VOCs and provided compound-dependent SA estimates as a function of longitudinal distance down the river. For many VOCs, the quality of the agreement between the model-simulated and measured concentrations could be improved by simple adjustments of the model input parameters.

The results obtained in this study illustrate the great utility of SA concepts when seeking to (1) understand and identify the sources and sinks acting to determine location-dependent concentrations of contaminants in surface waters; and (2) determine potential courses of action for remediation and source reduction in an effort to lower VOC concentrations in streams. In general, this study illustrated (1) the considerable difficulty of quantifying correctly the locations and magnitudes of ground-water-related sources of contamination in streams; and (2) that model-based estimates of stream VOC concentrations are likely to be most accurate when the major sources are point sources or tributaries where the spatial extent and magnitude of the sources are tightly constrained and easily determined.

References

Ashworth, R.A., Howe, G.B., Mullins, M.E., and Rogers, T.N., 1988, Air-water partitioning coefficients of organics in dilute aqueous solutions: Journal of Hazardous Materials, v. 18, p. 25–36.

Avery, S.T., and Novak, P., 1978, Oxygen transfer at hydraulic structures: Journal of the Hydraulics Division-American Society of Civil Engineers, v. 104, p. 1521–1540.

Caplow, Theodore, Schlosser, Peter, and Ho, D.T., 2004, Tracer study of mixing and transport in the upper Hudson River with multiple dams: Journal of Environmental Engineering, v. 130, no. 12, p. 1498–1506.

Connor, B.F., Rose, D.L., Noriega, M.C., Murtagh, L.K., and Abney, S.A., 1998, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—determination of 86 volatile organic compounds in water by gas chromatography/mass spectrometry, including detections less than reporting limits: U.S. Geological Survey Open-File Report 97–829, 78 p.

de Lima, Virginia, and Olimpio, J.C., 1989, Hydrogeology and simulation of ground-water flow at superfund site wells G and H, Woburn, Massachusetts: U.S. Geological Survey Water-Resources Investigations Report 89–4059, 99 p.

Gilliom, R.J., Alley, W.M., and Gurtz, M.E., 1995, Design of the National Water-Quality Assessment Program—occurrence and distribution of water-quality conditions: U.S. Geological Survey Circular 1112, 33 p.

Gossett, J.M., 1987, Measurement of Henry's Law constants for C1 and C2 chlorinated hydrocarbons: Environmental Science & Technology, v. 21, p. 202–208.

Gulliver, J.S., Wilhelms, S.C., and Parkhill, K.L., 1998, Predictive capabilities in oxygen transfer at hydraulic structures: Journal of Hydraulic Engineering-American Society of Civil Engineers, v. 124, p. 664–671.

Hall, G., and Watt, J.M., 1976, Modern numerical methods for ordinary differential equations: New York, Clarendon Press, Oxford University, 336 p.

Leighton, D.T., and Calo, J.M., 1981, Distribution coefficients of chlorinated hydrocarbons in dilute air-water systems for

groundwater contamination applications: Journal of Chemical and Engineering Data, v. 26, no. 4, p. 382–385.

Liss, P.S., and Slater, P.G., 1974, Fluxes of gases across the air-sea interface: Nature, v. 247, p. 181–184.

Lopes, T.J., and Price, C.V., 1997, Study plan for urban stream indicator sites of the National Water-Quality Assessment Program: U.S. Geological Survey Open-File Report 97–25, 15 p.

McLachlan, M., Mackay, D., and Jones, P.H., 1990, A conceptual model of organic-chemical volatilization at waterfalls: Environmental Science and Technology, v. 24, p. 252–257.

Mueller, D.K., Martin, J.D., and Lopes, T.J., 1997, Quality-control design for surface-water sampling in the National Water-Quality Assessment Program: U.S. Geological Survey Open-File Report 97–223, 17 p.

O'Conner, D.J., and Dobbins, W.E., 1958, Mechanism of reaeration in natural streams: Transactions American Society of Civil Engineers, v. 123, p. 641–666.

Owens, M., Edwards, R.W., and Gibbs, J.W., 1964, Some reaeration studies in streams: International Journal of Air and Water Pollution, v. 8, p. 469–486.

Pankow, J.F., Asher, W.E., and Zogorski, J.S., 2006, Source apportionment modeling of volatile organic compounds in streams: Environmental Toxicology and Chemistry, v. 25, no. 4, p. 921–932.

Pankow, J.F., Luo, Wentai, Bender, D.A., Isabelle, L.M., Hollingsworth, J.S., Chen, C., Asher, W.E., and Zogorski, J.S., 2003, Concentrations and co-occurrence correlations of 88 volatile organic compounds (VOCs) in the ambient air of 13 semi-rural to urban locations in the United States: Atmospheric Environment, v. 37, p. 5023–5046.

Pankow, J.F., Luo, Wentai, Isabelle, L.M., Bender, D.A., and Baker, R.J., 1998, Determination of a wide range of volatile organic compounds (VOCs) in ambient air using multisorbent adsorption/thermal desorption (ATD) and gas chromatography/mass spectrometry (GC/MS): Analytical Chemistry, v. 70, no. 24, p. 5213–5221.

Rathbun, R.E., 2000, Transport, behavior, and fate of volatile organic compounds in streams: Critical Reviews in Environmental Science & Technology, v. 30, p. 129–295.

Reid, R.C., Prausnitz, J.M., and Poling, B.E., 1987, The properties of gases and liquids (4th ed.): New York, McGraw-Hill, 741 p.

Rindels, A.J., and Gulliver, J.S., 1991, Oxygen transfer at spillways, *in* Wilhelms, S.C., and Gulliver, J.S., eds., Air-water mass transfer: Reston, Va., American Society of Civil Engineers, p. 524–533.

Robbins, G.A., Wang, Suya, and Stuart, J.D., 1993, Using the static headspace method to determine Henry's Law constants: Analytical Chemistry, v. 65, no. 21, p. 3113–3118.

Shelton, L.R., 1997, Field guide for collecting samples for analysis of volatile organic compounds in stream water for the National Water-Quality Assessment Program: U.S. Geological Survey Open-File Report 97–401, 20 p.

Urban, A.L., Hettiarachchi, S.L., Miller, K.F., Kincaid, G.P., and Gulliver, J.S., 2001, Field experiments to determine gas transfer at gated sills: Journal of Hydraulic Engineering-American Society of Civil Engineers, v. 127, p. 848–859.

Wanninkhof, R., 1992, Relationship between wind speed and gas exchange over the ocean: Journal of Geophysical Research, v. 97, p. 7373–7382.

Wanninkhof, R., Ledwell, J., and Crusius, J., 1991, Gas transfer velocities on lakes measured with sulfur hexafluoride, *in* Wilhelms, S.C., and Gulliver, J.S., eds., Air-water mass transfer: Reston, Va., American Society of Civil Engineers, p. 524–533.

Wilhelms, S.C., 1988, Reaeration at low-head gated structures—preliminary data: U.S. Army Corp of Engineers, Waterways Experiment Station, Vicksburg, Water Operations Technical Support Information Exchange Bulletin No. E–88–1, 4 p.

Wilke, C.R., and Chang, P., 1955, Correlation of diffusion coefficients in dilute solutions: American Institute of Chemical Engineering Journal, v. 1, p. 264–270.

Zhou, X., and Mopper, K., 1990, Apparent partition coefficients of 15 carbonyl compounds between air and seawater and between air and freshwater—implications for air-sea exchange: Environmental Science & Technology, v. 24, p. 1864–1869.

Appendixes

Appendix 1. FORTRAN Code for StreamVOC Model

```fortran
program streamvoc
  use msflib
  use dflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  character*255 aboutmessage
  integer i4, i
  logical lret
  external parfilin, Enviro_Params, CalcFlowProfile
!
!  Initialise Winteracter and open the main window.
!  This will also activate the main menu for the program.
!
  call WInitialise(' ')
  wc%flags  = SysMenuOn + MinButton + MaxButton
  wc%x      = -1
  wc%y      = -1
  wc%width  = 0
  wc%height = 0
  wc%menuid = IDR_MENU1
  wc%title  = 'StreamVOC - VOC Source Apportionment in Streams and Rivers'
  call WindowOpen(wc)
  call WBitmapGet(MainWinBitmap,0)
  aboutmessage = 'StreamVOC\nVersion 2.20:  April 10, 2004\n&
Includes gas exchange, mixing, biochemical degradation\n&
Gas exchange at weirs/sills [Gulliver et al. 1998]\n&
Component flux method for SA calculation\n\n&
William Asher\nOHSU-OGIST-EBS\nBeaverton, Oregon'C    !217 characters 4/12/04
!* This is the main loop of the program.  It does nothing but
!* cycle endlessly, allowing the menus to be used.
  do
    call WMessage(itype, mainmessage)
!   Branch depending on type of message.
    select case (itype)
!   Menu Selection, activate dialog, bring to front if already active.
      case (MenuSelect)
        select case (mainmessage%value1)
          case (IDD_LoadParamFile)
            call ParFilIn(lret)
            if (ParamFileOK) call CalcFlowProfile
            if (ProfileWindowOpen) then
              focusprofile = 2
              call ViewRiverProfile(lret)
            endif
          case (IDD_SaveResults)
            call DatFilOut(lret)
          case (IDD_ViewVOCParams)
            call VOC_Params(lret)
          case (IDD_EnviroParams)
             call Enviro_Params(lret)
          case (IDD_HydrogParams)
             call Hydrog_Params(lret)
          case (IDD_RuntimeParameters)
             call Model_Params(lret)
          case (IDD_ViewProfile)
             call ViewRiverProfile(lret)
          case (IDD_StartModel)
             call Start_Model(lret)
          case (IDD_HaltModel)
             call Halt_Model(lret)
          case (IDD_AboutBox)
            msg1 = 'About StreamVOC'
```

```
              call wmessagebox (OKOnly, InformationIcon, CommonOK, &
aboutmessage, msg1)
              call WindowSelect(0)
              call WBitmapPut(MainWinBitmap, 0, 0)
              if (ErrorWindow) then
                call WindowSelect(ErrWinUnit)
                call WBitmapPut(ErrWinBitmap, 0, 0)
              endif
              if (ProfileWindowOpen) then
                focusprofile = 2
                call ViewRiverProfile(lret)
              endif
            case (IDD_Exit)
              exit
          end select
        case (PushButton)
          select case (mainmessage.value1)
            case (ID_OKEnvParams)
              call Enviro_OK()
            case (ID_HydrogOK)
              call Hydrog_OK()
            case (ID_OKVOCParams)
              call VOCParam_OK()
            case (ID_OKModelParams)
              call ModelPar_OK()
          end select
!       Redisplay plot if we get an expose or resize event
        case (Expose,Resize)
          if (mainmessage.win .eq. 0) then
            if (.not. lrunning) then
              call WindowSelect(0)
              call WBitmapPut(MainWinBitmap, 0, 0)
            endif
          elseif (mainmessage.win .eq. ErrWinUnit) then
            if (ErrorWindow) then
              call WindowSelect(ErrWinUnit)
              call WBitmapPut(ErrWinBitmap, 0, 0)
            endif
          elseif (mainmessage.win .eq. ProfileWinUnit) then
            if (ProfileWindowOpen) then
              focusprofile = 2
              call ViewRiverProfile(lret)
            endif
          endif
        case (CloseRequest)
          if (mainmessage.win .eq. 0) then  ! closed main window, exit program
            exit
          elseif (mainmessage.win .eq. ErrWinUnit) then
            call WindowCloseChild(ErrWinUnit)
            ErrorWindow = .false.
          elseif (mainmessage.win .eq. ProfileWinUnit) then
            call WindowCloseChild(ProfileWinUnit)
            ProfileWindowOpen = .false.
          endif
      end select
    end do
    call WindowClose()
end
```

Begin StreamVOC Subroutines and Functions, Listed Alphabetically

```
subroutine CalcFlowProfile()
  use msflib
  use voccom
  implicit none
  integer  ipnts, i, j, k, n, imax, ierr, idist, icnt, iweir
```

```
   real*8 deltaflow, delx, xval, xmid, tempwid, makeup, &
         cfactor, q, ramp, offset
   real*8 fdw, inputinterp, GetSourceNumber, WeirEffic_Calc
   external fdw, inputinterp, GetSourceNumber, WeirEffic_Calc
   real*8 temparr(:,:)
   allocatable temparr
! FlowVolumes contains flow, width, depth info as function of distance
   if (allocated(FlowVolumes)) deallocate(FlowVolumes)
   ierr = iaxes + 2
   allocate (FlowVolumes(ierr, 2+4*Reaches+4*DistributedSources))
!  need distance, VOCInput, and SourceNumber for VOCInputs, that's why
!  it is dimensioned as iaxes+1
   if (allocated(VOCInputs)) deallocate(VOCInputs)
   ierr = iaxes + 1
   allocate (VOCInputs(ierr, 2+4*Reaches+4*DistributedSources))
! set data into array, FlowVolumes
! primary data array for river physical profile!
   FlowVolumes(1,1) = RiverData(1,1)    !distance   km
   FlowVolumes(2,1) = RiverData(1,5)    !flow volume    m^3/sec
   FlowVolumes(3,1) = RiverData(1,3)    !depth     m
   FlowVolumes(4,1) = RiverData(1,4)    !width     m
   imax = 1
   do j = 2, reachpoints-1
     if (RiverData(j,1) .eq. RiverData(j,2)) then
!      dealing with Reach endpoint or pnt. src.
!      if Reach boundary isn't there from dist source
!      need to add a point to FlowVolumes
       if (RiverData(j,1) .gt. FlowVolumes(1,imax)) then
!        increment IMAX to the new point
         imax = imax + 1
!        add in the point for the end of the reach
         FlowVolumes(1,imax) = RiverData(j,1)
         FlowVolumes(2,imax) = FlowVolumes(2,imax-1)
         FlowVolumes(3,imax) = FlowVolumes(3,imax-1)
         FlowVolumes(4,imax) = FlowVolumes(4,imax-1)
       endif
!      set the ramp distance =  river width up to a maximum of 5 m
       if (RiverData(j,4) .gt. 5.0d0) then
         ramp = 5.0d-3
       else
         ramp = 1.0d-3* RiverData(j,4)
       endif
!       increment IMAX to the new point
       imax = imax + 1
!       now add in all the changes in Flow, Depth, Width
       FlowVolumes(1,imax) = RiverData(j,1) + ramp
       FlowVolumes(2,imax) = FlowVolumes(2,imax-1) + RiverData(j,5)  !flow
       FlowVolumes(3,imax) = RiverData(j,3)                          !depth
       FlowVolumes(4,imax) = RiverData(j,4)                          !dwidth
     else
!      RiverData(j,1) .lt. RiverData(j,2) dist. source
!      find out if Dist Src starts at beginning of reach
!      (FlowVolumes(1,imax) is the last point,
!      either pnt src, reach boundary, or dist src)
       if (RiverData(j,1) .gt. FlowVolumes(1,imax)) then
!        start of new dist. src beyond last endpoint, add in start point
         imax = imax + 1
         FlowVolumes(1,imax) = RiverData(j,1)
         FlowVolumes(2,imax) = FlowVolumes(2,imax-1)  ! no change in flow
         FlowVolumes(3,imax) = FlowVolumes(3,imax-1)  ! no change in depth
         FlowVolumes(4,imax) = FlowVolumes(4,imax-1)  ! no change in width
       else
!        dist src starts before the last endpoint, nothing needs to be done
!        else here in case we change method and need it later
         continue
       endif
!      now add in point for dist src endpoint
```

```fortran
        imax = imax + 1
        FlowVolumes(1,imax) = RiverData(j,2)
        FlowVolumes(2,imax) = FlowVolumes(2,imax-1) + RiverData(j,5)
!      add the total increase in flow
        FlowVolumes(3,imax) = FlowVolumes(3,imax-1)   ! no change in depth
        FlowVolumes(4,imax) = FlowVolumes(4,imax-1)   ! no change in width
      endif
    end do
! add on the end point if necessary
! (may already be there if last dist. source ends at end of river)
    if (RiverData(ReachPoints,1) .gt. FlowVolumes(1,imax)) then
      imax = imax + 1
      FlowVolumes(1,imax) = RiverData(j,1)
      FlowVolumes(2,imax) = FlowVolumes(2,imax-1)
      FlowVolumes(3,imax) = FlowVolumes(3,imax-1)
      FlowVolumes(4,imax) = FlowVolumes(4,imax-1)
    endif
! now resize the array to be the correct number of elements
    ProfilePoints = imax
    ierr = iaxes+2
    allocate (temparr(ierr,ProfilePoints))
    do i = 1, ierr
      do j = 1, ProfilePoints
        temparr(i,j) = FlowVolumes(i,j)
      end do
    end do
    deallocate (FlowVolumes)
    allocate(FlowVolumes(ierr,ProfilePoints))
    do i = 1, ierr
      do j = 1, ProfilePoints
        FlowVolumes(i,j) = temparr(i,j)
      end do
    end do
    deallocate (temparr)
! now compute the VOC input profile
    VOCInputs(1,1) = RiverData(1,1)
    VOCInputs(2,1) = 0.0d0
    if (RiverData(1,6) .gt. 0.0d0) then
      VOCInputs(3,1) = 1
      SourceNumber = 1
!   next source will be the second, 1 is initial concentration
    else
      VOCInputs(3,1) = 0
      SourceNumber = 0
!   next source will be the first, no initial concentration
    endif
    imax = 1
    idist = 1
! CFACTOR converts m3*ug/sec-L into g/sec so that div by m.w. gives mol/sec
    cfactor = 1.0d-3
    do i = 2, reachpoints - 1
!   this if-then checks to make sure there is actually a source to include
      if ((RiverData(i,5) .gt. 0.0d0) .and. (RiverData(i,6) .gt. 0.0d0)) then
!     increment the source number to get ready for the next source
        SourceNumber = SourceNumber + 1
!     figure out if we have a distributed or point source
        if (RiverData(i,1) .lt. RiverData(i,2)) then
!       dealing with distributed source
          if (RiverData(i,1) .gt. VOCInputs(1,imax)) then
!         beginning is not at reach boundary
!         set the initial zero level for the new src
            imax = imax + 1
            VOCInputs(1,imax) = RiverData(i,1)
            VOCInputs(2,imax) = 0.0d0
            VOCInputs(3,imax) = SourceNumber
!         increment imax to add new point for src
            imax = imax + 1
```

```
!          set the source strength as the source beginning
           VOCInputs(1,imax) = RiverData(i,1)
!          see p-51 of STREAMVOC notebook for discussion
           VOCInputs(2,imax) = cfactor * RiverData(i,5) * RiverData(i,6) / &
                   (molweight * (1.0d3*(RiverData(i,2)-RiverData(i,1))))
           VOCInputs(3,imax) = SourceNumber
!          set the source strength at the source end
!          increment imax to add new point for src
           imax = imax + 1
           VOCInputs(1,imax) = RiverData(i,2)
           VOCInputs(2,imax) = cfactor * RiverData(i,5) * RiverData(i,6) / &
                   (molweight * (1.0d3*(RiverData(i,2)-RiverData(i,1))))
           VOCInputs(3,imax) = SourceNumber
!          bring the source back to zero
!          increment imax to add end point for src
           imax = imax + 1
           VOCInputs(1,imax) = RiverData(i,2)
           VOCInputs(2,imax) = 0.0d0
           VOCInputs(3,imax) = SourceNumber
         else    ! RiverData(j,1)<VOCInputs(1,imax) and sources overlap
!          because beginning of dist src is end of old one
!          don't need to add zero point
!          it's already there from previous point
!          just need to add point(s) for source strength
!          set the source strength at the beginning of the source
           imax = imax + 1
           VOCInputs(1,imax) = VOCInputs(1,imax-1)
!          see p-51 of STREAMVOC notebook for discussion
!          note that src distance adjusted for previous src. boundary
           VOCInputs(2,imax) = cfactor * RiverData(i,5) * RiverData(i,6) / &
                   (molweight * (1.0d3*(RiverData(i,2)-VOCInputs(1,imax))))
           VOCInputs(3,imax) = SourceNumber
!          set the source strength at the end of the source
           imax = imax + 1
           VOCInputs(1,imax) = RiverData(i,2)
           VOCInputs(2,imax) = cfactor * RiverData(i,5) * RiverData(i,6) / &
                   (molweight * (1.0d3*(RiverData(i,2)-VOCInputs(1,imax-1))))
!          change line above to IMAX-1 because incremented IMAX for new point
           VOCInputs(3,imax) = SourceNumber
!          now take the source input back to zero
           imax = imax + 1
           VOCInputs(1,imax) = RiverData(i,2)
           VOCInputs(2,imax) = 0.0d0
           VOCInputs(3,imax) = SourceNumber
         endif
       else
!        end of distributed source entry
!        RiverData(i,1) .eq. RiverData(i,2): confluence
         if (RiverData(i,1) .gt. VOCInputs(1,imax)) then
!          if there was no distributed source or end not at boundary
!          add in zero point
           imax = imax + 1
           VOCInputs(1,imax) = RiverData(i,1)
           VOCInputs(2,imax) = 0.0d0
           VOCInputs(3,imax) = SourceNumber
         endif
!        set the nominal src distance for a point source = max 5 m or width
         if (RiverData(i,4) .gt. 5.0d0) then
           ramp = 5.0d-3
         else
           ramp = 1.0d-3 * RiverData(i,4)
         endif
!         see p-51 of STREAMVOC notebook for discussion
         imax = imax + 1
         VOCInputs(1,imax) = VOCInputs(1,imax-1)
!        either way, this distance will be correct
!        set the source strength at the start of the source
```

```fortran
          VOCInputs(2,imax) = &
              cfactor*(RiverData(i,5)*RiverData(i,6))/(1.0d3*ramp*molweight)
          VOCInputs(3,imax) = SourceNumber
!         now add in the end of the point source RAMP distance after start
          imax = imax + 1
          VOCInputs(1,imax) = VOCInputs(1,imax-1) + ramp
          VOCInputs(2,imax) = &
              cfactor*(RiverData(i,5)*RiverData(i,6))/(1.0d3*ramp*molweight)
          VOCInputs(3,imax) = SourceNumber
!         add the final zero point bringing source to end
          imax = imax + 1
          VOCInputs(1,imax) = VOCInputs(1,imax-1)
          VOCInputs(2,imax) = 0.0d0
          VOCInputs(3,imax) = SourceNumber
        endif   ! end of reach boundary input
      endif     ! end of if-then to make sure there is actually a source
    end do
! add in the endpoint of the river, just in case
    VOCInputs(1,imax+1) = RiverLength
    VOCInputs(2,imax+1) = 0.0d0
    VOCInputs(3,imax+1) = 0.0d0
    VOCInputPoints = imax+1
! now resize the array to be the correct number of elements
    ierr = iaxes + 1
    allocate (temparr(ierr,VOCInputPoints))
    do i = 1, ierr
      do j = 1, VOCInputPoints
        temparr(i,j) = VOCInputs(i,j)
      end do
    end do
    deallocate (VOCInputs)
    allocate(VOCInputs(ierr,VOCInputPoints))
    do i = 1, ierr
      do j = 1, VOCInputPoints
        VOCInputs(i,j) = temparr(i,j)
      end do
    end do
    deallocate (temparr)
! now calculate lookup table for flow velocities
! to be used for timescales and transfer coefficients
! FLOWVELOCITY array defined in VOCCOM as (2,splinepnts), real*8
    MaxVelocity = 0.0d0
    MinVelocity = 500.0d0
    MaxVOCInput = 0.0d0
! deallocate the splined arrays if necessary
    if (allocated(spl_Depth)) deallocate(spl_Depth)
    if (allocated(spl_Width)) deallocate(spl_Width)
    if (allocated(spl_Flow)) deallocate(spl_Flow)
    if (allocated(spl_VOCInputs)) deallocate(spl_VOCInputs)
    if (allocated(spl_Veloc)) deallocate(spl_Veloc)
    if (allocated(spl_Timestep)) deallocate(spl_Timestep)
    if (allocated(spl_xval)) deallocate(spl_xval)
    if (allocated(OldData)) deallocate(OldData)
! figure out how many splined points we're going to need.
! Formula is on P-55 of STREAMVOC notebook 1 and is based on VOCInput array
    splinepnts = Boxpnts * (ProfilePoints - 1)
! allocate splined arrays
    allocate(spl_Depth(splinepnts))
    allocate(spl_Width(splinepnts))
    allocate(spl_Flow(splinepnts))
    allocate(spl_VOCInputs(3,splinepnts))
    allocate(spl_Veloc(2,splinepnts))
    allocate(spl_Timestep(splinepnts))
    allocate(spl_xval(splinepnts))
! reset splinepnts to 0 so that we have correct number of pnts
    splinepnts = 0
    icnt = 1
```

```fortran
  if (WeirNum .gt. 0) then
    iweir = 1
  else
    iweir = 0
  endif
  do i = 1, ProfilePoints-1
    delx = (FlowVolumes(1,i+1) - FlowVolumes(1,i)) / (dble(float(Boxpnts-1))) !   delx in km
    do j = 1, Boxpnts
      xval = FlowVolumes(1,i) + delx * float(j-1)    ! xval in km
      if ((xval .gt. spl_xval(icnt-1)) .or. (xval .eq. 0.0d0)) then
        xmid = xval + 0.5d0 * delx      !xmid in km
        if (xmid .gt. RiverLength) xmid = RiverLength
        spl_Depth(icnt) = fdw(xval,3)
        spl_Width(icnt) = fdw(xval,4)
        spl_Flow(icnt) = fdw(xval,2)  !  flow in m^3/sec
        spl_VOCInputs(1,icnt) = xval  !  calculates VOC input
        spl_VOCInputs(2,icnt) = inputinterp(xval)  ! VOC input in mol/(sec-m)
        spl_VOCInputs(3,icnt) = GetSourceNumber(xval)
!       flow is in m^3/s so velocity in m/s  is flow/(depth(m)*width(m))
!       calculate midpoint velocity as average over interval
        spl_Veloc(1,icnt) = xval
!       calculates midpoint flow velocity and other variables
        spl_Veloc(2,icnt)=fdw(xval,2)/(fdw(xval,3)*fdw(xval,4))
!       timestep is distance in km divided by velocity in m/sec * 0.001 km/m
!       1000 m/km * km * sec/m = sec
        spl_Timestep(icnt) = 1.0d3 * delx / spl_Veloc(2,icnt)
!       save the beginning xvalue of each interval, spl_xval is in km!
        spl_xval(icnt) = xval    ! xval in km
        if ((iweir .gt. 0) .and. (iweir .le. WeirNum)) then
          if (spl_xval(icnt) .ge. WeirPoints(iweir,1)) then
!           calculate specific flow
            q = spl_flow(icnt)/WeirPoints(iweir,2)
            WeirEffic(iweir) = WeirEffic_Calc(WeirType(iweir), q, &
              WeirPoints(iweir,3), WeirPoints(iweir,4), WeirPoints(iweir,5))
            iweir = iweir + 1
          endif
        endif
        if (spl_Veloc(2,icnt) .gt. MaxVelocity) &
            MaxVelocity = spl_Veloc(2,icnt)
        if (spl_Veloc(2,icnt) .lt. MinVelocity) &
            MinVelocity = spl_Veloc(2,icnt)
        if (spl_VOCInputs(2,icnt) .gt. MaxVOCInput) &
            MaxVOCInput = spl_VOCInputs(2,icnt)
        if (spl_VOCInputs(2,icnt) .lt. MinVOCInput) &
            MinVOCInput = spl_VOCInputs(2,icnt)
        icnt = icnt + 1
        splinepnts = splinepnts+1
      endif
    end do !j
  end do !i
!  debugging output used to write the Splined Data sets
!  open (10, file = 'test.dat')
!  write(10, '(a,a)') '      xval        depth       width    flow',&
!  '      x-VOCInput    y-VOCInput    x-Veloc       y-Veloc      Timestep'
!  do i = 1, splinepnts
!    write (10, '(5f12.4,e14.4,f10.1,f12.4,2e14.4)') spl_xval(i), &
!      spl_Depth(i), spl_Width(i), spl_Flow(i),
!      (spl_VOCInputs(j,i), j = 1, 3), (spl_Veloc(j,i), j = 1, 2), &
!      spl_Timestep(i)
!  end do
!  close(10)
! end debugging output
! allocate data array used for plotting data when model runs
  allocate(OldData(2,splinepnts,2))
  return
end subroutine CalcFlowProfile
```

```fortran
subroutine cfunc_comp (t, c, dt)
! CFUNC partitions net flux into Fin and Fout
! Fin = kOA * Cs
! Fout = kOA * Cb
! P125 of River Modelling I lab notebook
  use VOCCOM
  use cfunccom
  implicit none
! local real*8 variables, some are shorthand notation
  integer i
  real*8 t,c(num_eqs),dt(num_eqs), mtinv,dmi, dmiair, dmt, gasout, gasin, &
         airterm, gwloss, area
  real*8 sourceinput(:)
  allocatable sourceinput
  allocate (sourceinput(num_eqs))
  ! c(1) = River flow (m^3/sec)
  ! c(2) = River concentration (mol/m^3)
  ! c(3:num_eqs-1) = concentration fractions of the individual sources
  ! c(num_eqs) = air source conc. fractopm
  ! dt(1) = dQ/dt
  ! dt(2) = dC(total)/dt
  ! dt(3:num_eqs-1) = change in conc. frac. of the individual sources
  ! dt(num_eqs) = change in conc frac of air source
  area = c(1) / depth
  gasout = kl*area*c(2)
  gasin = kl*area*cs
  dt(1) = qprime
! GWLOSS removes VOC mass from river due to flow to groundwater
  if (qprime .lt. 0.0d0) then
    gwloss = qprime * c(2)   ! remove mass if necessary
  else
    gwloss = 0.0d0           ! remember to reset to zero if not needed
  endif
  dt(2) = (gasin - gasout + ii + gwloss)/c(1) - kd*c(2) - c(2)*dt(1)/c(1)
  mtinv = 1.0d0 / (c(1) * c(2))
  dmt = (gasin - gasout - kd*c(2)*c(1) + ii + gwloss)
  sourceinput = 0.0d0   ! array initialization
! need to add two to currentsource to offset for flow and total concentration
  sourceinput(currentsource+2) = ii
  sourceinput(num_eqs) = gasin
  do i = 3, num_eqs     ! i = num_eqs is the atmospheric source
    dmi = sourceinput(i) + c(i) * (gwloss - gasout - kd*c(2)*c(1))
!   change in concentration fraction
    dt(i) = mtinv * (dmi - c(i)*dmt)
  end do
  deallocate (sourceinput)
  return
end subroutine cfunc_comp

subroutine cfunc_net (t, c, dt)
! version of CFUNC that does not partition net flux into Fin and Fout
! does not calculate atmospheric source term if Cs <= Cb
! used in versions of StreamVOC that are pre-June 23, 2005
  use VOCCOM
  use cfunccom
  implicit none
! local real*8 variables, some are shorthand notation
  integer i
  real*8 t, c(num_eqs), dt(num_eqs), mtinv,dmi,dmiair,dmt,gasex,airterm, &
         gwloss, area
  real*8 sourceinput(:)
  allocatable sourceinput
  allocate (sourceinput(num_eqs))
  ! c(1) = River flow (m^3/sec)
  ! c(2) = River concentration (mol/m^3)
  ! c(3:num_eqs-1) = concentration fractions of the individual sources
  ! c(num_eqs) = air source conc. fractopm
```

```
  ! dt(1) = dQ/dt
  ! dt(2) = dC(total)/dt
  ! dt(3:num_eqs-1) = change in conc frac of the individual sources
  ! dt(num_eqs) = change in conc frac of air source
  area = c(1) / depth
  gasex = kl*area*(cs-c(2))
  dt(1) = qprime
! removes VOC mass from river due to loss of flow to groundwater
  if (qprime .lt. 0.0d0) then
    gwloss = qprime * c(2)    ! remove mass if necessary
  else
    gwloss = 0.0d0            ! remember to reset to zero if not needed
  endif
  dt(2) = (gasex + ii + gwloss)/c(1) - kd*c(2) - c(2)*dt(1)/c(1)
  mtinv = 1.0d0 / (c(1) * c(2))
  dmt = (gasex - kd*c(2)*c(1) + ii + gwloss)
  do i = 3, num_eqs
    sourceinput(i) = 0.0d0
  end do
! need to add two to currentsource to offset for flow and total conc
  sourceinput(currentsource+2) = ii
  if (gasex .gt. 0.0d0) then
    airterm = 0.0d0    ! source from atmosphere
    dmiair = gasex + c(num_eqs)*(-kd*c(2)*c(1) + gwloss)
  else
    airterm = gasex    ! sink to atmosphere
    dmiair = c(num_eqs)*(gasex-kd*c(2)*c(1) + gwloss)
  endif
! i = num_eqs is the atmospheric source term, dealt with separately
  do i = 3, num_eqs-1
    dmi = sourceinput(i) + c(i) * (airterm - kd*c(2)*c(1) + gwloss)
!   change in conc frac defined on page 68 of StreamVOC notebook 1
    dt(i) = mtinv * (dmi - c(i)*dmt)
  end do
  dt(num_eqs) = mtinv * (dmiair - c(num_eqs)*dmt)
  deallocate (sourceinput)
  return
end subroutine cfunc_net

real*8 function cs_func(i)
! calculates csat from water temperature
use VOCcom
implicit none
integer numpts, i
real*8 t, time, atmpr, deg_c, airconc, interpolate, sol_calc, local_sol
external interpolate
deg_c = SurfaceTemp
airconc = AtmVOCConc
atmpr = AtmosPress
airconc = airconc * 1.0d-9   !  change ppbv into atmospheres
local_sol = sol_calc(deg_c, SolParam)  !  solubility in mol/m^3-atm
cs_func = local_sol * airconc * atmpr
return
end function cs_func

subroutine DatFilOut(bool_in)
! saves the output data file from the model
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  logical ret, bool_in
  integer ierror
  character*255 Datfile_Out_tmp
  character*60 dlgtitle
  call unusedqq(checked)
```

```fortran
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(ret)
    endif
    return
  endif
!* dialog title
  dlgtitle = 'Save Model Output to ASCII File'
!  reset temporary filename
  Datfile_Out_tmp = ''
!* create dialog
  call WSelectFile(IDS_DataFileString, 13, Datfile_Out_tmp, dlgtitle)
!* check for error
  VOC_File_Sav = .false.
  if (Datfile_Out_tmp .ne. '') then
    Datfile_Out = Datfile_Out_tmp
    call save_VOC(VOC_File_Sav)
  endif
  return
end subroutine DatFilOut

real*8 function diff_calc(tempc, iform)
! function returns D in cm^2/sec which is converted to Sc for calculating kL
! nu used in Sc relation is also cm^2/sec so no need to convert D to SI units
use VOCcom
implicit none
integer iform
real*8 tempc
real*8 mu, nu, sc
select case (iform)
  case(1)
!   Absolute viscosity (mu) in gm-cm/sec calc. from temperature in deg-C.
!   The underlying data is from data from CRC 63rd edition.
!   The polynomial fit was done in the spreadsheet KINVISC.WB1 in QDATA
    mu = 1.7825047d0-5.75921d-2*tempc+1.11378d-3*tempc**2-9.55317d-6*tempc**3
    diff_calc = (4.7199d-07*(tempc+2.7316d2))/(mu*(MolarVolume**0.6d0))
  case(2)
    sc = wd0 + wd1*tempc + wd2*tempc**2 + wd3*tempc**3
!   Kinematic viscosity (nu) in cm^2/sec is calc. from temperature in deg-C.
!   The underlying data is from data from CRC 63rd edition.
!   The polynomial fit was done in the spreadsheet KINVISC.WB1 in QDATA
    nu=1.7826598d-2-5.76464d-4*tempc+1.12266d-5*tempc**2-9.66507d-8*tempc**3
    diff_calc = 0.0d0
    if (sc .ne. 0.0d0) diff_calc = nu/sc
end select
return
end function diff_calc

subroutine dot2space(tline)
implicit none
character*72 tline
integer length, i
length = len_trim(tline)
do i = 1, length
  if (tline(i:i) .eq. '~') tline(i:i) = ' '
end do
return
end subroutine dot2space
```

```fortran
real*8 function dqdt(i)
! calculates derivative of flow volumes w.r.t. time using flow_volume and velocity series
use voccom
implicit none
logical test
integer i
real*8 b, flow1, flow2
! begin subroutine
flow1 = spl_Flow(i)
flow2 = spl_Flow(i+1)
b = (flow2 - flow1) / spl_timestep(i)
dqdt = b
return
end function dqdt

subroutine Enviro_OK()
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  call WDialogUnload()
  menuactive = .false.
  return
end subroutine Enviro_OK

SUBROUTINE Enviro_Params(bool_in)
!***************************************************************************
!*                                                                        *
!*  This subroutine creates a dialog box that allows the user to view     *
!*  the parameters associated with the enviromental conditions.  It also  *
!*  sets the call back routines for the help and ok buttons.              *
!*                                                                        *
!***************************************************************************
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  logical lret, bool_in
  integer iret, ierr, iloop
  external Enviro_ok
  call unusedqq(bool_in)
  ierr = 0
  msg0 = ''
  msg1 = ''
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  iloop = 1
    menuactive = .true.
!   initialize the dialog box
    call WDialogLoad(IDD_EnviroParams)
!   write initial values and set subroutines
```

```
      if (iloop .eq. 1) then
        write(err_str(1), '(f7.2)') 100*Rel_Hum
        write(err_str(2), '(f7.2)') WindSpeed
        write(err_str(3), '(f7.2)') AirTemp
        write(err_str(4), '(f7.2)') AtmosPress
        write(err_str(5), '(f7.2)') SurfaceTemp
      endif
      call WDialogPutString(IDC_RelativeHumidity, err_str(1))
      call WDialogPutString(IDC_WindSpeed, err_str(2))
      call WDialogPutString(IDC_AirTemp, err_str(3))
      call WDialogPutString(IDC_AtmPressure, err_str(4))
      call WDialogPutString(IDC_WaterTemp, err_str(5))
!     initiate the dialog window
      call WDialogShow(-1, -1, 0, 2)  ! show modeless dialog IDD_EnviroParams
   return
end subroutine Enviro_Params

subroutine ErrorOutput(vpos, offset)
use msflib
use winteracter
use VOCcom
implicit none
integer vpos, offset
call WindowSelect(ErrWinUnit)
call WindowOutString(0, vpos, msg0)
vpos = vpos + offset
return
end subroutine ErrorOutput

real*8 function fdw(x, icol)
use VOCcom
integer numcols, icol
real*8 x
real*8 interpolate
external interpolate
numpts = ProfilePoints
numcols = 4
fdw = interpolate(FlowVolumes, x, icol, numcols, numpts)
return
end function fdw

real function findmaxval(index)
! index is column of RiverData array to find maximum value
use voccom
integer index, i
findmaxval = 0.0
do i = 1, ReachPoints
  if (findmaxval .lt. sngl(RiverData(i,index))) &
      findmaxval = sngl(RiverData(i,index))
end do
return
end function findmaxval

real*8 function flux_h2o(t)
!note:  flux_h2o unused in streamvoc, left in for future modeling of stream
!       evaporation
use VOCcom
real*8 t
real*8 airt, tempk, degc, logvp, vp, delc, time, u, ka_h2o, flux_mass
numpts = splinepnts
degc = SurfaceTemp
u = WindSpeed
airt = AirTemp
! variable T is time in days from model start, TIME is time in months
time = 1.2d1*(t/3.65d2 - float(int(t/3.65d2)))
! Air-side resistance estimated from H2O relation in Schwarzenbach et al. Env. Org. Chem.
```

```fortran
ka_h2o = 0.01d0*(0.2d0*u+0.3d0)*dsqrt((airt+2.7316d2)/2.9316d2)          !ka_h2o in m/s at
AirTemp
tempk = degc + 2.7316d2
! v.p. of H2O predicted from data from CRC-63rd, fit done in Quattro
logvp = 3.14004128517d1 + -6.788619575d1*(1.0d2/tempk) + -5.00162020852d0*dlog(1.0d-2*tempk)
vp = dexp(logvp)
vpatm = vp/7.60d2
delc = (1.0d0 - rel_hum) * vpatm / (gasconst * tempk) ! delta-C for water
flux_mass = 2.4d1 * 3.6d3 * 1.8d1 * ka_h2o * delc ! water lost in g/day-m^2
flux_h2o = 1.0d-03 * flux_mass  ! height of water loss in mm over timestep
return
end function flux_h2o

real*8 function GetSourceNumber(x)
use VOCcom
integer numcols, numpts, i, icol
real*8 x, VOCin
real*8 interpolate
external interpolate
numpts = VOCInputPoints
numcols = 3
icol = 2
VOCin = interpolate(VOCInputs, x, icol, numcols, numpts)
if (VOCin .gt. 0.0d0) then
  i = 1
  do while (i .le. numpts-1)
    if ((x .ge. VOCInputs(1,i)) .and. (x .le. VOCInputs(1,i+1))) then
      GetSourceNumber = max(VOCinputs(3,i), VOCInputs(3,i+1))
      return
    endif
    i = i + 1
  end do
endif
GetSourceNumber = 0
return
end function GetSourceNumber

subroutine go_vocdrv(arg2)
!*****************************************************************************
!*                                                                          *
!*  description for subroutine go_vocdrv(arg2)                              *
!*                                                                          *
!*  used to call the subroutine that does the modeling calculations        *
!*                                                                          *
!*****************************************************************************
  use dfmt
  implicit none
  integer(4) arg2
  arg2 = 0
  call vocdrv
  call exitthread(0)     !exit code is 0
  return
end subroutine go_vocdrv

SUBROUTINE Halt_Model(bool_in)
! halts model in mid-run, processing may continue until stop is reached in
! rkintout.for
  use msflib
  use winteracter
  use voccom
  implicit none
  logical(kind=4) bool_in
  integer iret
  call unusedqq(bool_in)
  lrunning = .false.
  menuactive = .false.
  return
end subroutine Halt_Model
```

```fortran
subroutine Hydrog_OK()
!***************************************************************************
!*  callback routine for when the ok button has been pushed               *
!***************************************************************************
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  call WDialogUnload()
  menuactive = .false.
  return
end subroutine Hydrog_OK

subroutine Hydrog_Params(bool_in)
  use msflib
  use winteracter
  use voccom
  implicit none
  INCLUDE 'RESOURCE.FD'
  character*128 dialogtext(:)
  allocatable dialogtext
  integer i, j, iret, index
  logical bool_in, lret
  call unusedqq(bool_in)
  allocate (dialogtext(reachpoints))
  msg0 = ''
  msg1 = ''
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  menuactive = .true.
! initialize the dialog box
  call WDialogLoad(IDD_HydrogParamsList)
  write(err_str(1),'(i5)') Reaches
  write(err_str(2),'(f13.2)') RiverLength
  write(err_str(3),'(i5)') DistributedSources
  index = 3
  do i = 1, ReachPoints
    if (RiverData(i,1) .eq. RiverData(i,2)) then
      iret = 1    ! reach boundary
    else
      iret = 2    ! distributed source
    endif
    if (i .lt. 10) then
      write(dialogtext(i), '(2x,i4,10x,i1,2x,6(5x, e11.4),6x,i4)') &
          i, iret, (RiverData(i,j), j=1,6), int(RiverData(i,7))
    elseif ((i .ge. 10) .and. (i .lt. 100)) then
      write(dialogtext(i), '(1x,i4,10x,i1,2x,6(5x, e11.4),6x,i4)') &
          i, iret, (RiverData(i,j), j=1,6), int(RiverData(i,7))
    else
      write(dialogtext(i), '(i4,10x,i1,2x,6(5x, e11.4),6x,i4)') &
          i, iret, (RiverData(i,j), j=1,6), int(RiverData(i,7))
    endif
```

```
   end do
   index = index + ReachPoints
   call WDialogPutMenu(IDC_HydrogParamList, dialogtext, reachpoints, 1)
   call WDialogPutString(IDC_ReachPoints, err_str(1))
   call WDialogPutString(IDC_TotalLength, err_str(2))
   call WDialogPutString(IDC_DistributedSourcePoints, err_str(3))
! bring up the dialog box
   call WDialogShow(-1, -1, 0, 2)
   deallocate (dialogtext)
   return
end subroutine Hydrog_Params

real*8 function inputinterp(x)
use VOCcom
integer numcols, icol
real*8 x
real*8 interpolate
external interpolate
numpts = VOCInputPoints
numcols = 3
icol = 2
i = 1
inputinterp = interpolate(VOCInputs, x, icol, numcols, numpts)
return
end function inputinterp

real*8 function interpolate(x_series, xval, icol, numcols, numpts)
! interpolation routine for SPLINEPNT-pt time series.
implicit none
integer i, numpts, iday, numcols, icol
real*8 x_series(numcols,numpts), xi, xf, yi, yf, xval
i = 1
do while (i .le. numpts)
  if (xval .eq. x_series(1,i)) then
    interpolate = x_series(icol,i)
    return
  elseif ((xval .gt. x_series(1,i)) .and. (xval .le. x_series(1,i+1))) then
    xi = x_series(1,i)
    xf = x_series(1,i+1)
    yi = x_series(icol,i)
    yf = x_series(icol,i+1)
    interpolate = yi + (yf-yi)*((xval-xi)/(xf-xi))
    return
  endif
  i = i + 1
end do
return
end function interpolate

real*8 function kd_func(i)
! function calculates the biochemical degradation rate of the VOC
use VOCcom
implicit none
integer numpts, i
real*8 ii_kgday, t, time
!, interpolate
!external interpolate
! now just sets kd_func equal to degradation rate since constant but used a
!function in case I want to change to make a function of time
kd_func = DegradationRate
return
end function kd_func

real*8 function kl_func(i)
! calculates kL from river flow velocity, water depth, water temperature, &
! and wind speed
! Calculates Koa assuming liquid and gas-phase rate control
```

```
! Based opn relationships contained in &
! USGS Paper 1589, Transport, Behavior, and fate of Volatile
! Organic Compounds in Streams by D. Rathbun.  pp4-12 & pp 35-40
use VOCcom
implicit none
integer numpts, i
real*8 airt, kl_mps, depth, u, v, degc, sc, diff_calc, nu, phi, psi, &
       ka_h2o_26, k20, kltemp, kvoc, ka_voc, kl_voc, kH, sol_calc, d
external diff_calc, sol_calc
u = WindSpeed
degc = SurfaceTemp
airt = AirTemp
v = spl_veloc(2,i)
depth = spl_depth(i)
kH = sol_calc(degc, SolParam)
d = diff_calc(degc, DiffParam)          !  calculate diffusivity (d) of VOC
!   Kinematic viscosity (nu) in cm^2/sec is calculated from temp in deg-C.
!   The underlying data is from data from CRC 63rd edition.
!   The polynomial fit was done in the spreadsheet KINVISC.WB1 in QDATA
nu = 1.7826598d-2-5.76464d-04*degc+1.12266d-05*degc**2-9.66507d-08*degc**3
sc = nu/d
! Air-side resistance estimated from H2O relation on P 57 of Rathbun, Eq. 57,
! Temp corr using Eq. 58 and refer to VOC using Eqs. 26 and 28
ka_h2o_26 = (4.16d2 + 1.56d2*u)/(2.4d1*3.6d3)     !eq. 57, ka_h2o in m/day @ 26.1 deg-C converted
to m/s
psi = 4.42d0 * MolWeight**(-0.462d0)          ! Eq. 28, correction factor
! correct ka @26 C for H2O to VOC at air temperature
ka_voc = psi * ka_h2o_26 * exp(9.34d-3*(airt - 2.61d1))
! now do some conditional testing to set the correct range for
! parameterization for kL
if ((v .ge. 0.05d0) .and. (depth .gt. 0.274d0)) then
  ! Reaerat coeff K in 1/day from O'Conner & Dobbins (Eq. 55, Rathbun) 20 C
  k20 = 3.93d0 * sqrt(v) * depth**(-1.5d0) / (2.4d1*3.6d3)  ! eq. 55
  kvoc = k20 * (1.024d0)**(degc - 2.0d1)                    ! eq. 56
  phi = 2.52d0 * molarvolume**(-0.301d0)                    ! eq. 27
! eq. 25 and converted to m/sec from 1/sec as in Eq. 16
  kl_voc = depth * phi * kvoc
elseif ((v .ge. 0.04d0) .and. (depth .ge. 0.119d0)) then
  ! Reaer coeff K in 1/day from Owens et al. (Eq. 53, Rathbun) at 20 C
  k20 = 6.92d0 * (v**0.73d0) * depth**(-1.75d0) / (2.4d1*3.6d3)  ! eq. 55
  kvoc = k20 * (1.024d0)**(degc - 2.0d1)                    ! eq. 56
  phi = 2.52d0 * molarvolume**(-0.301d0)                    ! eq. 27
! eq. 25 and converted to m/sec from 1/sec as in Eq. 16
  kl_voc = depth * phi * kvoc
elseif (v .lt. 0.04d0) then
! neither flow formula works, calc kL using U since we are in a pond
! kL in m/s from Wanninkhof et al. (1991; GasEx2 symp. paper on Page 441)
  kl_voc = 0.01d0*0.45d0*dsqrt(600.0d0/sc)*u**1.64d0/3.6d3
endif
! if-then needed for kG param.  can't divide by zero for kl_voc at u=0
if ((u .eq. 0.0d0) .and. (v .lt. 0.04d0)) then
  ! no water-side term, only kA
  kl_mps = ka_voc/(kH*gasconst*(degc+273.16d0))
else
  kl_mps=1.0d0/(1.0d0/kl_voc+1.0d0/(ka_voc/(kH*gasconst*(degc+273.16d0))))
endif
kl_func = kl_mps ! set value for kOL to the function output
return
end function kl_func

real*8 function mass_input(i)
! function calculates the VOC input
use VOCcom
implicit none
integer numpts, i
real*8 delx
! this makes sure we don't multiply a big xvalue times a voc input per meter
```

```
! it really screws up the mass balance
! delx is in km
if (i .gt. 1) then
  delx = min((spl_xval(i+1) - spl_xval(i)), (spl_xval(i) - spl_xval(i-1)))
else
  delx = (spl_xval(i+1) - spl_xval(i))
endif
! spl_VOCInputs is in mol/sec-m so 1.0d3 changes delx(km) to delx(m)
mass_input = 1.0d3 * spl_VOCInputs(2,i+1) * delx / spl_timestep(i)
return
end function mass_input

integer function mass_source(i)
! function calculates the VOC input to the lake from motorboats etc.
use VOCcom
implicit none
integer numpts, i
mass_source = max(int(spl_VOCInputs(3,i)), int(spl_VOCInputs(3,i+1)))
return
end function mass_source

subroutine menuset(ival)
use msflib
use winteracter
use VOCcom
implicit none
include 'resource.fd'
integer ival
! ival = 1: enable   ival = 0: grayed
  call WMenuRoot(IDR_Menu1)
  call WMenuSetState(IDD_SaveResults,1,ival)    ! VOC_Params enabled
  call WMenuSetState(IDD_ViewVOCParams,1,ival)    ! VOC_Params enabled
  call WMenuSetState(IDD_EnviroParams,1,ival)    ! Enviro_params enabled
  call WMenuSetState(IDD_HydrogParams,1,ival)    ! Hyrog_params enabled
  call WMenuSetState(IDD_RuntimeParameters,1,ival)    ! Model_params enabled
  call WMenuSetState(IDD_ViewProfile,1,ival)    ! View_River_Profile
  call WMenuSetState(IDD_StartModel,1,ival)    ! Start_model enabled
  call WMenuSetState(IDD_HaltModel,1,ival)    ! Start_model enabled
return
end subroutine menuset

subroutine menusetrunning(ival)
use msflib
use winteracter
use VOCcom
implicit none
include 'resource.fd'
integer ival
! ival = 1: enable   ival = 0: grayed
  call WMenuRoot(IDR_Menu1)
  call WMenuSetState(IDD_LoadParamFile,1,ival)    ! Load param disabled
  call WMenuSetState(IDD_SaveResults,1,ival)    ! Save_data disabled
  call WMenuSetState(IDD_ViewVOCParams,1,ival)    ! VOC_Params disabled
  call WMenuSetState(IDD_EnviroParams,1,ival)    ! Enviro_params disabled
  call WMenuSetState(IDD_HydrogParams,1,ival)    ! Hyrog_params disabled
  call WMenuSetState(IDD_RuntimeParameters,1,ival)    ! Model_params disabled
  call WMenuSetState(IDD_ViewProfile,1,ival)    ! View_River_Profile
  call WMenuSetState(IDD_StartModel,1,ival)    ! Start_model disabled
  call WMenuSetState(IDD_HaltModel,1,1)        ! Halt model enabled
  call WMenuSetState(IDD_AboutBox,1,ival)    ! About Box
return
end subroutine menusetrunning

subroutine Model_Params(bool_in)
  use msflib
  use winteracter
  use voccom
```

```fortran
  implicit none
  include 'resource.fd'
  logical lret, err, bool_in
  integer iret
  call unusedqq(bool_in)
  msg0 = ''
  msg1 = ''
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  err = .true.
  menuactive = .true.
! initialize the dialog box
  call WDialogLoad(IDD_RuntimeParams)
  write(err_str(2),'(i4)') Boxpnts
  write(err_str(3),'(e15.4)') Tolerance
  err_str(4) = Title
  err_str(5) = Comment(1)
  err_str(6) = Comment(2)
  call WDialogPutString(IDC_NumberOfBoxes, err_str(2))
  call WDialogPutString(IDC_Tolerance, err_str(3))
  call WDialogPutString(IDC_Title, err_str(4))
  call WDialogPutString(IDC_Comment1, err_str(5))
  call WDialogPutString(IDC_Comment2, err_str(6))
! bring up the dialog box
  call WDialogShow(-1, -1, 0, 2)
  return
end subroutine Model_Params

subroutine ModelPar_OK ()
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  call WDialogUnload()
  menuactive = .false.
  return
end subroutine ModelPar_OK

subroutine openerrorwindow
use voccom
use winteracter
if (errorwindow) then
  call WindowRaise(ErrWinUnit)
  call WindowClear()
else
  errorwindowwc%flags  = SysMenuOn + MinButton + MaxButton
  errorwindowwc%x      = 20
  errorwindowwc%y      = 50
  errorwindowwc%width  = 600
  errorwindowwc%height = 800
  errorwindowwc%menuid = 0
  errorwindowwc%title  = 'StreamVOC_Winteracter Parameter File Input Errors'
```

```
  call WindowOpenChild(errorwindowwc, ErrWinUnit)
  errorwindow = .true.
endif
return
end subroutine openerrorwindow

subroutine parfilin(bool_in)
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  logical ret, ts_error, bool_in
  integer ierror, i
  character*255 Parfile_In_TMP
  character*60 dlgtitle
  external read_parfile
  call unusedqq(bool_in)
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(ret)
    endif
    return
  endif
! the next 7 lines added to automatically read data from default.par
!  ret = .true.
!  ierror = 0
!  if(ret .and. (ierror == 0))then
!    Parfile_In = 'default.par'
!    call read_parfile
!  endif
!  return
! remove before production version
  dlgtitle = 'Read Parameter File'
  Parfile_In_TMP = ''
  call WSelectFile(IDS_ParameterFileString, 8, Parfile_In_TMP, dlgtitle)
  if (Parfile_In_TMP .ne. '') then
    Parfile_In = Parfile_In_TMP
    call read_parfile
  endif
end subroutine ParFilIn

subroutine PlotProfile(xleft, xright, ybottom, ytop, deltay, xmin, xmax, &
  ymin,ymax,xdata,ydata1,ydata2,numpnts,numsets,colorvalue,xlabel,ylabel)
integer numpnts, numsets, colorvalue, iticks, strlen
parameter (iticks = 5)
real*4 xdata(numpnts), ydata1(numpnts), ydata2(numpnts)
real*4 xleft, xright, ybottom, ytop, deltay, xmin, xmax, ymin, ymax
real*4 xticks(iticks), yticks(iticks)
character*(*) xlabel, ylabel
  call IGrArea(xleft, ytop-deltay, xright, ytop)
  call IGrUnits(xmin, ymin, xmax, ymax)
  call IPgArea(0.1, 0.15, 0.95, 0.95)
  call IPgNewGraph(numsets, numpnts, '', '', 'X')
  call IPgStyle(1, 0, 0, 0, colorvalue, colorvalue)
! see col256 in wint/demos for key to values
  if (numsets .eq. 2) call IPgStyle(2, 0, 0, 0, colorvalue, colorvalue)
```

```fortran
  call IPgUnits(xmin, ymin, xmax, ymax)
! set the x-axis ticks
  call SetTicks(xticks, iticks, xmin, xmax)
! set the y-axis ticks
  call SetTicks(yticks, iticks, ymin, ymax)
  call IGrCharFont(7)
  call IGrCharSize(1.0, 2.0)
  call IPgXScalePos(0.45)
  call IPgXUserScale(xticks, iticks)
  call IPgYUserScale(yticks, iticks)
  call IPgAxesXY(xmin, ymin)
  call IPgXTickPos(ymin,ymax)
  call IPgXscale('TN')
  call IPgYscaleLeft('TN')
  call IPgXLabel(xlabel,'C')
  call IPgYLabelPos(0.6)
  call IPgYLabelLeft(ylabel,'B9')
  call IPgXYPairs(xData, yData1)
  if (numsets .eq. 2) call IPgXYPairs(xData, yData2)
return
end subroutine PlotProfile

subroutine read_parfile
subroutine read_parfile
  use msflib
  use winteracter
  use VOCcom
  implicit none
  include 'resource.fd'
  integer(kind=4) vpos, offset
  integer(kind=4)iret, i, ierror, ifile, j, isource
  logical lexist, error, f_error, data_ok, diffsol_error, la_error, &
          initialsettings, lret
  character*3 dbs
  character*72 dtitle, dcomment(2), header, error_msg
  character*255 tempfile, FileSave
  integer ipnts, isplit, dReachPoints, dReaches, dDistributedSources, idum,&
          dDiffParam, dSolParam, dWeirType(:), dWeirNum
  real*8 dRiverLength, dSurfaceTemp, dAtmVOCConc, dDegradationRate,dAirTemp,&
       dWindSpeed, dAtmosPress, dInitialFlowRate, dMolWeight, dTol, dMV, &
       dDensity, dSalinity, dsola, dsolb, dwa0, dwa1, dwa2, dwb0, dwb1, &
       dwb2, dwd0, dwd1, dwd2, dwd3, drel_hum, dRiverData(:,:), &
       dDiffusivity, dSolubility, dTimestep, dWeirPoints(:,:)
  real*8 tempc, sc, mu, nu, tempk, sol1, alpha, logalpha
  allocatable dRiverData, dWeirType, dWeirPoints
  external ParFilIn, DatFilOut, VOC_Params, Enviro_Params, Hydrog_Params,&
          Model_Params, Start_model, Halt_model, ViewRiverProfile
  data dbs/'$$$'/
  tempfile = '*.*'
!  set temp MolarVolume variable to -1 so we can see if it's been set already
! Need to do this because
  dMV = 1.0d0
  offset = 250
  vpos = 200
! first reset the error flag and close the error window (if open)
  error = .false.
  ierror = 0
!* open parameter file
  inquire (file=ParFile_In, exist=LExist)
  if (.not. LExist) then
    msg0 = ' Parameter file does not exist!\nRe-enter filename'C
    msg1 = ' ERROR OPENING FILE '
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
```

```
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  if (allocated(dRiverData)) deallocate(dRiverData)
  if (allocated(dWeirPoints)) deallocate(dWeirPoints)
  if (allocated(dWeirType)) deallocate(dWeirType)
  open (ParFilUnit, file=ParFile_In, status='OLD', action = 'READ')
! read in header line, then the ModelFunction switch:
!               1 for Component Fluxes, 0 for net fluxes
  ModelFunction = -1
  WeirFlow = -1
  FlowUnits = -1
  read (ParFilUnit, *, iostat=ifile)
  read (ParFilUnit, *, iostat=ifile) ModelFunction, WeirFlow, FlowUnits
  if ((ifile .ne. 0) .or. (ModelFunction .eq. -1) .or. &
      (WeirFlow .eq. -1) .or. (FlowUnits .eq. -1)) then
    error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write(msg0,'(a,i2,a)')'Input Error #',ierror,': Error Reading Flags'
    call ErrorOutput(vpos, offset)
  endif
  if ((ModelFunction .lt. 0) .and. (ModelFunction .gt. 1)) then
    error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
         ':  ModelFunction Flag must be 0 or 1'
    call ErrorOutput(vpos, offset)
  endif
  if ((WeirFlow .lt. 0) .and. (WeirFlow .gt. 1)) then
    error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
         ':  WeirFlow Flag must be 0 or 1'
    call ErrorOutput(vpos, offset)
  endif
  if ((FlowUnits .lt. 0) .and. (FlowUnits .gt. 1)) then
    error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
         ':  FlowUnits Flag must be 0 or 1'
    call ErrorOutput(vpos, offset)
  endif
! read in header line, then total river length (km)
  read (ParFilUnit, *, iostat=ifile)
  read (ParFilUnit, *, iostat=ifile) dRiverLength
  if (ifile .ne. 0) then
    error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
         ':  Error reading river length.'
    call ErrorOutput(vpos, offset)
  endif
! read in header line, then the number of reaches
  read (ParFilUnit, *, iostat=ifile)
  read (ParFilUnit, *, iostat=ifile) dReaches
  if (ifile .ne. 0) then
    error = .true.
```

```
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading reach points.'
      call ErrorOutput(vpos, offset)
    endif
! read in header line, then number of distributed source regions
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dDistributedSources
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading distributed source points.'
      call ErrorOutput(vpos, offset)
    endif
! calculate the number reach points to be read in (=dReaches+dDistSources+1)
    dReachPoints = dReaches + dDistributedSources + 1
    if (dReachPoints .gt. 101) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Sum of # of reaches & dist. sources must be <= 100 '
      call ErrorOutput(vpos, offset)
    endif
! allocate river data array in preparation for reading in river physical data
    allocate (dRiverData(dReachPoints, 6))
! read in the two header lines, then read the river physical data into dRiverData array
! #  StartDist. (km) EndDist.(km)  Depth(m)  Width(m)  Flow(cfm)  Conc.(ug/L)
! for distributed source, flow is total increase over source region
! for distributed source, concentration is average conc. over source region
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile)
    do i = 1, dReachPoints
      read (ParFilUnit, *, iostat=ifile) idum, (dRiverData(i,j), j = 1, 6)
      if (ifile .ne. 0) then
        error = .true.
        ierror = ierror + 1
        if (ierror .eq. 1) call OpenErrorWindow
        write (msg0, '(a,i2,a,i2)') 'Input Error #', ierror, &
              ':  Error reading reach data point #', i
        call ErrorOutput(vpos, offset)
      endif
    end do
! read in header line, then river temperature (C)
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dSurfaceTemp
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading river temperature.'
      call ErrorOutput(vpos, offset)
    endif
! read in header line, then air temperature (C)
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dAirTemp
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading air temperature.'
      call ErrorOutput(vpos, offset)
```

```
     endif
! read in header line, then wind speed (m/s)
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) dWindSpeed
   if (ifile .ne. 0) then
     error = .true.
     ierror = ierror + 1
     if (ierror .eq. 1) call OpenErrorWindow
     write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
             ':  Error reading wind speed.'
     call ErrorOutput(vpos, offset)
   endif
! read in header line, then relative humidity
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) drel_hum
   if (ifile .ne. 0) then
     error = .true.
     ierror = ierror + 1
     if (ierror .eq. 1) call OpenErrorWindow
     write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
             ':  Error reading relative humidity.'
     call ErrorOutput(vpos, offset)
   endif
! read in header line, then barometric pressure (atm)
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) dAtmosPress
   if (ifile .ne. 0) then
     error = .true.
     ierror = ierror + 1
     if (ierror .eq. 1) call OpenErrorWindow
     write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
             ':  Error reading atmospheric pressure.'
     call ErrorOutput(vpos, offset)
   endif
! read in header line, then atmos. VOC concentration (ppbv)
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) dAtmVOCConc
   if (ifile .ne. 0) then
     error = .true.
     ierror = ierror + 1
     if (ierror .eq. 1) call OpenErrorWindow
     write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
             ':  Error reading atmospheric VOC concentration.'
     call ErrorOutput(vpos, offset)
   endif
! read in header line, then VOC molec. weight (g/mol)
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) dMolWeight
   if (ifile .ne. 0) then
     error = .true.
     ierror = ierror + 1
     if (ierror .eq. 1) call OpenErrorWindow
     write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
             ':  Error reading atmospheric pressure.'
     call ErrorOutput(vpos, offset)
   endif
! read in header line, then diffusivity parameterization
! 1 for Wilke-Chang (requires molar volume at normal boiling point)
! 2 for Wanninkhof polynomial fit
   read (ParFilUnit, *, iostat=ifile)
   read (ParFilUnit, *, iostat=ifile) dDiffParam
   read (ParFilUnit, *, iostat=ifile)
   if (dDiffParam .eq. 1) then
!    read in VOC molar volume at normal boiling point (mL/mol)
     read (ParFilUnit, *, iostat=ifile) dMV
     if (ifile .ne. 0) then
       error = .true.
```

```fortran
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading molar volume.'
      call ErrorOutput(vpos, offset)
    endif
  elseif (dDiffParam .eq. 2) then
!     read in VOC density in g/mL
    read (ParFilUnit, *, iostat=ifile) dDensity
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
            ':  Error reading VOC density.'
      call ErrorOutput(vpos, offset)
    endif
  else
    error = .true.
    diffsol_error = .true.
    ierror = ierror + 1
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Diffusivity parameterization .ne. (1 .or. 2).'
    call ErrorOutput(vpos, offset)
  endif
! read in header line, then solubility parameterization
! 1 for exp(-(A-B/T))
! 2 for Wanninkhof polynomial fit
! 3 for direct entry
  read (ParFilUnit, *, iostat=ifile)
  read (ParFilUnit, *, iostat=ifile) dSolParam
  read (ParFilUnit, *, iostat=ifile)
  if (dSolParam .eq. 1) then
!     read in VOC molar volume at normal boiling point (ml/mol)
    read (ParFilUnit, *, iostat=ifile) dSolA, dSolB
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading exponential solubility coefficients.'
      call ErrorOutput(vpos, offset)
    endif
  elseif (dSolParam .eq. 2) then
!     read in four wanninkhof Sc parameterization coefficients
    read (ParFilUnit,*,iostat=ifile)dwa0,dwa1,dwa2,dwb0,dwb1,dwb2,dSalinity
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading Wanninkof solubility coefficients.'
      call ErrorOutput(vpos, offset)
    endif
  elseif (dSolParam .eq. 3) then
!   read in solubility directly
    read (ParFilUnit, *, iostat=ifile) dSolubility
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading solubility.'
      call ErrorOutput(vpos, offset)
    endif
  else
```

```
      error = .true.
      diffsol_error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Solubility parameterization .ne. (1 .or. 2 .or. 3).'
      call ErrorOutput(vpos, offset)
    endif
! read in header line, then degradation rate (1/sec)
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dDegradationRate
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading VOC degradation rate.'
      call ErrorOutput(vpos, offset)
    endif
! read in header line, then tolerance for Runge-Kutta
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dTol
    if (ifile .ne. 0) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading Runge-Kutta tolerance.'
      call ErrorOutput(vpos, offset)
    endif
! read title, comment line header and read title and comments, if they exist
    read (parfilunit, *, iostat=ifile)
    title = '        '
    if (ifile .eq. 0) then
      read (parfilunit, '(72a)', iostat=ifile) dtitle
      if (ifile .eq. 0) then
        read (parfilunit, '(72a)', iostat=ifile) dcomment(1)
        if (ifile .eq. 0) then
          read (parfilunit, '(72a)', iostat=ifile) dcomment(2)
        endif
      endif
    endif  ! End of comment line input
!  read in the weir/waterfall information
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile)
    read (ParFilUnit, *, iostat=ifile) dWeirNum
    if ((ifile .ne. 0) .or. (dWeirNum .lt. 0)) then
      error = .true.
      ierror = ierror + 1
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0, '(a,i2,a)') 'Input Error #', ierror, &
          ':  Error reading number of weir points.'
      call ErrorOutput(vpos, offset)
    endif
! check to see if there are any weirs, if not, go on to check for errors
    if (dWeirNum .gt. 0) then
! allocate river data array in preparationfor reading in river physical data
      allocate (dWeirPoints(dWeirNum,5))
      allocate (dWeirType(dWeirNum))
!    read in the weir information
! #  WeirLocation (km)  L(width)  h  s  Ht  WeirType
!    (see WeirEffic in physicchem.f90 for details)
      read (ParFilUnit, *, iostat=ifile)
      read (ParFilUnit, *, iostat=ifile)
      do i = 1, dWeirNum
        read (ParFilUnit, *, iostat=ifile) idum, (dWeirPoints(i,j), j=1,5), &
            dWeirType(i)
```

```fortran
      if (ifile .ne. 0) then
        error = .true.
        ierror = ierror + 1
        if (ierror .eq. 1) call OpenErrorWindow
        write (msg0, '(a,i2,a,i2)') 'Input Error #', ierror, &
         ':  Error reading reach data point #', i
        call ErrorOutput(vpos, offset)
      endif
    end do
  endif
!  end of weir input information
! read in data output filename if present
  read (ParFilUnit, *, iostat=ifile) tempfile
! close the parameter file, end of data input.
  close (parfilunit)
  ierror = 0
  if (.not. error) then
    if (dRiverLength .le. 0.0d0) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a)')
      ' Error in RIVER LENGTH.  Length must be > 0'
      call ErrorOutput(vpos, offset)
    endif
    if (dRiverData(dReachPoints,1) .ne. dRiverLength) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a,a)') ' Error in river physical data.  ',&
            'Maximum length must be = Total River Length'
      call ErrorOutput(vpos, offset)
    endif
    if (dMolWeight .le. 0.0d0) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a)')
      ' Error in MOLECULAR WEIGHT.  Weight must be >0'
      call ErrorOutput(vpos, offset)
    endif
    if (dSurfaceTemp .lt. 0.0d0) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a)') &
          ' Error in river temperature.  Temperature must be > 0.0 C'
      call ErrorOutput(vpos, offset)
    endif
    if (dAirTemp .le. -50.0d0) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a)') &
         ' Error in AIR TEMPERATURE.  Air Temp must be > -50 C'
      call ErrorOutput(vpos, offset)
    endif
    if (dDegradationRate .lt. 0.0d0) then
      ierror = ierror + 1
      error = .true.
      if (ierror .eq. 1) call OpenErrorWindow
      write (msg0,'(a)')
      ' Error in DEGRADATION RATE.  Rate must be >= 0.0 1/s'
      call ErrorOutput(vpos, offset)
    endif
    if (dWindSpeed .le. 0.0d0) then
      ierror = ierror + 1
```

```
          error = .true.
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in WIND SPEED.  WIND SPEED must be >= 0'
          call ErrorOutput(vpos, offset)
        endif
        if ((drel_hum .le. 0.0d0) .or. (dRel_Hum .gt. 100.0)) then
          ierror = ierror + 1
          error = .true.
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in RELATIVE HUMIDITY.  0 .GE. RH .LE. 100'
          call ErrorOutput(vpos, offset)
        endif
        if (dAtmosPress .le. 0.0d0) then
          ierror = ierror + 1
          error = .true.
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in ATMOSPHERIC PRESSURE.  PRESSURE must be .GT. 0'
          call ErrorOutput(vpos, offset)
        endif
        if (dAtmVOCConc .lt. 0.0d0) then
          ierror = ierror + 1
          error = .true.
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in ATMOS, VOC CONCENTRATION.  CONCENTRATION must be .GE. 0'
          call ErrorOutput(vpos, offset)
        endif
        if (dTol .le. 0.0d0) then
          ierror = ierror + 1
          error = .true.
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in TOLERANCE.  TOLERANCE must be .GT. 0'
          call ErrorOutput(vpos, offset)
        endif
        if (dRiverData(1,1) .ne. 0.0d0) then
          error = .true.
          ierror = ierror + 1
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in river physical data point # 1, distance .NE. 0.0'
          call ErrorOutput(vpos, offset)
        endif
        if ((dRiverData(1,3) .le. 0.0d0) .or. (dRiverData(1,4) .le. 0.0d0) .or. &
            (dRiverData(1,6) .lt. 0.0d0)) then
          error = .true.
          ierror = ierror + 1
          if (ierror .eq. 1) call OpenErrorWindow
          write (msg0,'(a)')
          ' Error in river phys. data point # 1, depth, width, or conc. <= 0.0'
          call ErrorOutput(vpos, offset)
        endif
        do i = 2, dReachPoints - 1
          if (dRiverData(i,1) .lt. dRiverData(i-1,2)) then
!           Distance must increase from end to beginning points
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a, i2, a)') &
              ' Error in river physical data point #', i, ' distance decreases'
            call ErrorOutput(vpos, offset)
          endif
          if (dRiverData(i,2) .lt. dRiverData(i,1)) then
            error = .true.
```

```fortran
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a, i2, a)') ' Error in data point #', i+1, &
                 ' distances decrease from start-end'
            call ErrorOutput(vpos, offset)
          endif
          if ((dRiverData(i,2)-dRiverData(i,1) .gt. 0.0d0) .and. &
              (dRiverData(i,2)-dRiverData(i,1) .lt. &
                        1.0d-3*min(5.0d0, dRiverData(i,4)))) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a, i2, a)') ' Error in data point #', i+1, &
                 ' dist. src length too small'
            call ErrorOutput(vpos, offset)
          endif
          if ((dRiverData(i,3).le.0.0d0).or.(dRiverData(i,4).le.0.0d0)) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') ' Error in river physical data point #',i,&
              ' depth or width <= 0.0'
            call ErrorOutput(vpos, offset)
          endif
          if (dRiverData(i,3) .le. 0.119d0) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') ' Error in river physical data point #',i,&
                 ' depth <= 0.119 m, cannot parameterize kL'
            call ErrorOutput(vpos, offset)
          endif
          if (dRiverData(i,6) .lt. 0.0d0) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') 'Error in river physical data point #',i,&
               ' conc < 0.0'
            call ErrorOutput(vpos, offset)
          endif
          if ((dRiverData(i,1) .lt. dRiverData(i,2)) .and. &
              (dRiverData(i,6) .lt. 0.0d0)) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') 'Error in river physical data point #',i,&
                 'distributed source conc < 0.0'
            call ErrorOutput(vpos, offset)
          endif
        end do
!    now check the weir data, if there is any
      if (dWeirNum .gt. 0) then
        do i = 1, dWeirNum
          if ((dWeirType(i) .lt. 1) .or. (dWeirType(i) .gt. 3)) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') ' Error in weir #', i, &
               '  invalid weir type (1, 2, or 3)'
            call ErrorOutput(vpos, offset)
          endif
          if ((dWeirPoints(i,1) .le. 0.0d0) .or. &
              (dWeirPoints(i,1) .ge. dRiverLength)) then
            error = .true.
            ierror = ierror + 1
            if (ierror .eq. 1) call OpenErrorWindow
            write (msg0,'(a,i2,a)') ' Error in weir #', i, '  invalid position'
```

```
        call ErrorOutput(vpos, offset)
      endif
    end do
  endif
!  now check diffusivity and solubility for validity (both must be > 0)
  if (dDiffParam .eq. 2) then
    dMV = dDensity / dMolWeight
  endif
  tempc = dSurfaceTemp
!  Absolute viscosity (mu) in gm-cm/sec is calc. from temper in deg-C.
!  The underlying data is from data from CRC 63rd edition.
!  The polynomial fit was done in the spreadsheet KINVISC.WB1 in QDATA
  mu=1.7825047d0-5.75921d-2*tempc+1.11378d-3*tempc**2-9.55317d-06*tempc**3
  if (dMV .gt. 0.0d0) then
    dDiffusivity = (4.7199d-07*(tempc+2.7316d2))/(mu*(dMV**0.6d0))
  else
    dDiffusivity = -1.0d0
  endif
  if (dDiffusivity .le. 0.0d0) then
    ierror = ierror + 1
    error = .true.
    if (ierror .eq. 1) call OpenErrorWindow
    write (msg0,'(a)')
    ' Error in Diffusivity or parameterization.  Diffusivity must be > 0'
    call ErrorOutput(vpos, offset)
  endif
  if (dDiffusivity .gt. 0.1) then
!     diffusivity of VOC in water>larger than diffus. of heat
    error_msg = 'Parameter File Warning'
    msg0 = &
   'Calculated Diffusivity > 1.0 cm^2/sec!\nPlease check parameter file'C
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, error_msg)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      call WindowSelect(ProfileWinUnit)
      call WindowFontColour(NotSet, TextWhiteBold)
      call WindowClearArea(0,0,9999,9999)
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
  endif
  select case (dSolParam)
    case (1, 2)
      tempk = dSurfaceTemp + 2.7315d2
      if (dSolParam .eq. 1) then
        dSolubility = 1.0d0/dexp(dsolA - dsolB/(tempk))
!       following Robbins et al., mol/m^3-atm
      else
!        calculating Bunsen solubilities assuming salinity = zero
!        using Wanninkhof relation
        logalpha = dwa0 + dwa1*(1.0d2/tempk) + dwa2*dlog(1.0d-2*tempk) + &
          dsalinity * (dwb1 + dwb2*(1.0d-2*tempk) + dwb2*(1.0d-2*tempk)**2)
        alpha = dexp(logalpha)
        sol1 = alpha /(8.20575d-2 * (tempk))   ! mol/L-atm
        dSolubility = 1.0d3*sol1                ! mol/m^3-atm
      endif
    case (3)
      continue
  end select
  if (dSolubility .le. 0.0d0) then
    ierror = ierror + 1
    error = .true.
```

```fortran
      if (ierror.eq.1) open(ErrWinUnit,file='USER',title='PARAM FILE ERRORS')
      write (msg0,'(a)')
      ' Error in Solubility or parameterization.  Solubility must be > 0'
      call ErrorOutput(vpos, offset)
    endif
    if (0.001*dSolubility .gt. 100.0) then
      error_msg = 'Parameter File Warning'
      msg0 = &
    'Calculated Solubility > 100.0 mol/L-atm!\nPlease check parameter file'C
      call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, error_msg)
      call WindowSelect(0)
      call WBitmapPut(MainWinBitmap, 0, 0)
      if (ErrorWindow) then
        call WindowSelect(ErrWinUnit)
        call WBitmapPut(ErrWinBitmap, 0, 0)
      endif
      if (ProfileWindowOpen) then
        call WindowSelect(ProfileWinUnit)
        call WindowFontColour(NotSet, TextWhiteBold)
        call WindowClearArea(0,0,9999,9999)
        focusprofile = 2
        call ViewRiverProfile(lret)
      endif
    endif
!   Now check to make sure there aren't more than 25 sources or the data
!   output string will be longer than 255 characters and we'll get an error
    isource = 0
    do i = 1, ReachPoints
      if ((dRiverData(i,5) .gt. 0.0d0) .and. &
          (RiverData(i,6) .gt. 0.0d0)) then
        isource = isource + 1
      endif
    end do
    if (isource .gt. 25) then
      ierror = ierror + 1
      error = .true.
      if (ierror.eq.1) open(ErrWinUnit,file='USER',title='PARAM FILE ERRORS')
      write (msg0,'(a)')
      ' Too many sources.  Total number must be <= 25'
      call ErrorOutput(vpos, offset)
    endif
! now finally try to open the output data file if tempfile .ne. '*.*'
    if ((.not. error) .and. (tempfile .ne. '*.*')) then
      FileSave = DatFile_Out
      DatFile_Out = tempfile
      call Save_VOC
    endif
    if (.not. error) then
!   NEED TO RESET THE DIFFUS AND SOL COEFFICIENTS BEFORE RETURNING
      Density = dDensity
      MolarVolume = dMV
      sola = dsola
      solb = dsolb
      wa0 = dwa0
      wa1 = dwa1
      wa2 = dwa2
      wb0 = dwb0
      wb1 = dwb1
      wb2 = dwb2
      salinity = dsalinity
      DiffParam = dDiffParam
      SolParam = dSolParam
      Diffusivity = dDiffusivity
      Solubility = dSolubility
      rel_hum = drel_hum
      RiverLength = dRiverLength
      SurfaceTemp = dSurfaceTemp
```

```
      AtmVOCConc = dAtmVOCConc
      DegradationRate = dDegradationRate
      AirTemp = dAirTemp
      WindSpeed = dWindSpeed
      AtmosPress = dAtmosPress
      MolWeight = dMolWeight
      Tolerance = dTol
      ReachPoints = dReachPoints
      Reaches = dReaches
      DistributedSources = dDistributedSources
      Title = dTitle
      comment(1) = dcomment(1)
      comment(2) = dcomment(2)
      if (allocated(RiverData)) deallocate(RiverData)
      allocate(RiverData(ReachPoints,7))
      isource = 0
      do i = 1, ReachPoints
        do j = 1, 6
          RiverData(i,j) = dRiverData(i,j)
        end do
!      need to convert flow units if they were entered as cfm
        if (FlowUnits .eq. 1) then
!        Flow entered in param file as cfm so we need to convert to m^3/s
          RiverData(i,5) = dRiverData(i,5)/2118.9d0
        endif
        if ((RiverData(i,5) .gt. 0.0d0) .and. &
            (RiverData(i,6) .gt. 0.0d0)) then
          isource = isource + 1
          RiverData(i,7) = isource
        endif
      end do
      deallocate (dRiverData)
      if (dWeirNum .gt. 0) then
        WeirNum = dWeirNum
        if (allocated(WeirPoints)) deallocate(WeirPoints)
        if (allocated(WeirType)) deallocate(WeirType)
        if (allocated(WeirEffic)) deallocate(WeirEffic)
        allocate(WeirType(WeirNum))
        allocate(WeirPoints(WeirNum,5))
        allocate(WeirEffic(WeirNum))
        WeirType = dWeirType
        WeirPoints = dWeirPoints
      else
        WeirNum = 0
      endif
      if (allocated(dWeirPoints)) deallocate (dWeirPoints)
      call WindowSelect(0)
      call WBitmapPut(MainWinBitmap, 0, 0)
      call WindowFontColour(NotSet, TextWhiteBold)
      call WindowClearArea(0,0,9999,1900)
      msg0 = 'Parameter file successfully read'
      call WindowOutString(0, 300, msg0)
      msg0 = 'View input parameters enabled'
      call WindowOutString(0, 600, msg0)
      msg0 = 'Model ready to run'
      call WindowOutString(0, 900, msg0)
      call WBitmapGet(MainWinBitmap,0)
      if (ErrorWindow) then
        call WindowSelect(ErrWinUnit)
        call WBitmapPut(ErrWinBitmap, 0, 0)
      endif
      call menuset(1)  ! turn menus on
!      some housekeeping stuff
      OpenWindow = .true.    ! tells Plot subroutine to open graphics window
      ParamFileOK = .true.   ! successfuly read parameter file
      if (errorwindow) then
        call WindowCloseChild(ErrWinUnit)
```

```fortran
            errorwindow = .false.
          endif
          return
        else
          errorwindow = .true.
          msg0 = &
'Errors in param file!\nPlease check file\nErrors in error output window'C
          call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
          call WindowSelect(0)
          call WBitmapPut(MainWinBitmap, 0, 0)
          if (ErrorWindow) then
            call WindowSelect(ErrWinUnit)
            call WBitmapPut(ErrWinBitmap, 0, 0)
          endif
          if (ProfileWindowOpen) then
            call WindowSelect(ProfileWinUnit)
            call WindowFontColour(NotSet, TextWhiteBold)
            call WindowClearArea(0,0,9999,9999)
            focusprofile = 2
            call ViewRiverProfile(lret)
          endif
          ParamFileOK = .false.      ! parameter file not read
          call WBitmapGet(ErrWinBitmap,0)
          call menuset(0)  ! set menus off
          return
        endif
      else
        msg0='Errors in param file\nFILE NOT READ!!!!\nPlease check param file.'C
        call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
        call WindowSelect(0)
        call WBitmapPut(MainWinBitmap, 0, 0)
        if (ErrorWindow) then
          call WindowSelect(ErrWinUnit)
          call WBitmapPut(ErrWinBitmap, 0, 0)
        endif
        if (ProfileWindowOpen) then
          focusprofile = 2
          call ViewRiverProfile(lret)
        endif
        errorwindow = .true.
        ParamFileOK = .false.      ! successfuly read parameter file
        call WBitmapGet(ErrWinBitmap,0)
        call menuset(0)  ! set menus off
        return
      endif
end subroutine read_parfile

subroutine save_voc (forcewrite)
!saves an mtbe data file, checks to make sure existing file not overwritten.
  use msflib
  use winteracter
  use voccom
  implicit none
  logical forcewrite    !  if .true. then overwrite any existing file
  integer iret, ierr, ibutton
  integer*2 delval
  logical LExist, lret
!* open Data output file
  inquire (file=DatFile_Out, exist=LExist)
  if ((LExist) .and. (.not. forcewrite)) then
    msg0 = trim(DatFile_out)
    msg1 = ' OVERWRITE FILE? '
    call wmessagebox (YesNo, ExclamationIcon, CommonNo, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
```

```fortran
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    if (WInfoDialog(4) .eq. CommonYes) then
      delval = delfilesqq(DatFile_Out)
      ierr = 0
      open(DatFilUnit, file=DatFile_Out, status='NEW', iostat=ierr)
      if (ierr .ne. 0) then
        write(msg0, '(a,i3)') 'Unknown File I/O Error, IOSTAT value =', ierr
        msg1 = ' ERROR OPENING FILE '
        call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
        call WindowSelect(0)
        call WBitmapPut(MainWinBitmap, 0, 0)
        if (ErrorWindow) then
          call WindowSelect(ErrWinUnit)
          call WBitmapPut(ErrWinBitmap, 0, 0)
        endif
        if (ProfileWindowOpen) then
          focusprofile = 2
          call ViewRiverProfile(lret)
        endif
        return
      endif
      DatOut = .true.
      VOC_File_sav = .true.
    endif
  else
    if (LExist) delval = delfilesqq(DatFile_Out)
    ierr = 0
    open(DatFilUnit, file=DatFile_Out, status='NEW', iostat=ierr)
    if (ierr .ne. 0) then
      write(msg0, '(a,i3)')  ' Unknown File I/O Error, IOSTAT value = ', ierr
      msg1 = ' ERROR OPENING FILE '
      call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
      call WindowSelect(0)
      call WBitmapPut(MainWinBitmap, 0, 0)
      if (ErrorWindow) then
        call WindowSelect(ErrWinUnit)
        call WBitmapPut(ErrWinBitmap, 0, 0)
      endif
      if (ProfileWindowOpen) then
        focusprofile = 2
        call ViewRiverProfile(lret)
      endif
      return
    endif
    DatOut = .true.
    VOC_File_sav = .true.
  endif
  return
end subroutine save_voc

subroutine SetTicks (ticks, iticks, xmin, xmax)
implicit none
integer iticks
real*4 ticks(iticks), xmin, xmax
integer i
  do i = 1, iticks
    ticks(i) = xmin + (xmax-xmin) * float(i-1) / float(iticks-1)
    if (ticks(i) .gt. 1.0) then
      if (xmax .ge. 10.0) then
        ticks(i) = float(floor(ticks(i)))
!       make sure we plot ticks on even numbers
      else
```

```fortran
         ticks(i) = 0.1*float(floor(10.0*ticks(i)))
!        retain the tenth digit in the tick
         endif
      elseif (ticks(i) .gt. 0.10) then
        ticks(i) = 0.01*float(floor(100.0*ticks(i)))
!       round xticks(i) to the nearest tenth
      elseif (ticks(i) .gt. 0.010) then
        ticks(i) = 0.001*float(floor(1000.0*ticks(i)))
!       round xticks(i) to the nearest hundredth
!       add in more elseifs here if we decide to run river streams with
!       intervals smaller than a 0.01 m
      endif
  end do
return
end subroutine SetTicks

real*8 function sol_calc(tempc, iform)
use VOCcom
implicit none
integer iform
real*8 tempc
real*8 tempk, logalpha, alpha, sol1
tempk = tempc + 2.7316d2
select case (iform)
  case(1)
    sol_calc=1.0d0/dexp(solA-solB/(tempk)) ! from Robbins et al., mol/m^3-atm
  case(2)
!   calc Bunsen sol. assuming salinity = zero using Wanninkhof relation
    logalpha = wa0 + wa1*(1.0d2/tempk) + wa2*dlog(1.0d-2*tempk) + &
            salinity * (wb1 + wb2*(1.0d-2*tempk) + wb2*(1.0d-2*tempk)**2)
    alpha = dexp(logalpha)
    sol1 = alpha /(8.20575d-2 * (tempk))    ! mol/L-atm
    sol_calc = 1.0d3*sol1                    ! mol/m^3-atm
  case(3)
    sol_calc = solubility
end select
return
end function sol_calc

subroutine Start_Model(lret)
  use dfmt
  use msflib
  use winteracter
  use voccom
  implicit none
  integer(kind=4)iret
  external go_vocdrv
  integer(kind=4) arg2, threadhandle,threadid, i
  logical ts_error, lret
  ts_error = .false.
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore starting model'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  i = 1
```

```fortran
   if (.not. lrunning) then
     lrunning = .true.
     call WindowSelect(0)
     call WBitmapPut(MainWinBitmap, 0, 0)
     call WindowFontColour(NotSet, TextWhiteBold)
     call WindowClearArea(0,0,9999,1900)
     call WindowOutString(0, 300, title)
     call WindowOutString(0, 600, comment(1))
     call WindowOutString(0, 900, comment(2))
!  need to check file I/O before detach thread or it screws up graphics
     if (.not. DatOut) then
       msg0 = 'Model output will not be saved to data file'
     else
       msg0 = 'Model output saved to data file: '//trim(DatFile_out)
     endif
     call WindowOutString(0, 1300, msg0)
     msg1 = 'Model Status:  Running'
     call WindowOutString(0, 1600, msg1)
!  Note:  From DVF example CHAOS.F90 (Launch_ChaosDrive File:Lchchsdr.f90)
!  added the type LOC() around ARG2.  Keeps thread running.
     call menusetrunning(0)
     arg2=0
     threadhandle = createthread(0,0,go_vocdrv,loc(arg2),0,threadid)
   else
     call WindowFontColour(TextRedBold, TextWhiteBold)
     msg0 = &
' Model already running!   Press <Run\\Stop> to terminate before restarting'
     call WindowOutString(0, 1600, msg0)
     call WindowFontColour(TextBlack, TextWhiteBold)
   endif
   return
end subroutine Start_Model

subroutine ViewRiverProfile (bool_in)
   use msflib
   use winteracter
   use voccom
   implicit none
   integer id, callbacktype
   logical bool_in, lret
   integer  retcode, ipnts, i, j, k, ierr
   integer  iscale, iticks
! real constants needed by Winteracter (can't use real*8!)
   real xmin, xmax, ymin, ymax, xticks(5), yticks(5)
   real maxdepth, maxwidth, maxflow, minflow, findmaxval, vocmin, vocmax, &
       minvel, maxvel
   real xwindowleft, xwindowright, deltaywindow, yspacing, ylast
   real xDepth(:), yDepth1(:), yDepth2(:), yWidth1(:), yWidth2(:), yFlow(:), &
       yVelocity(:), xVOCInput(:), yVOCInput(:)
   allocatable xDepth, yDepth1, yDepth2, yWidth1, yWidth2, yFlow, &
       yVelocity, xVOCInput, yVOCInput
   external findmaxval
   call unusedqq(bool_in)
! set these data so they get reinitialized every time we call the subroutine
   xwindowleft = 0.0
   xwindowright = 1.0
   deltaywindow = 0.2
   yspacing = 0.0
   ylast = 1.0
   xmin = 0.0e0
   xmax = sngl(RiverLength)
   iticks = 5
! fill in the tickmark array for the x-axis
   do i = 1, iticks
     xticks(i) = sngl(RiverLength) * float(i-1) / float(iticks-1)
   end do
! allocate the temporary REAL*4 arrays used by Winteracter for data plotting
```

```fortran
     allocate (xDepth(ProfilePoints), yDepth1(ProfilePoints), &
               yDepth2(ProfilePoints), yWidth1(ProfilePoints), &
               yWidth2(ProfilePoints), yFlow(ProfilePoints), &
               yVelocity(ProfilePoints)), (xVOCInput(VOCInputPoints), &
               yVOCInput(VOCInputPoints))
! find the maximum depth and width
   maxdepth = findmaxval(3)   !  RiverData has depth in column 3
   maxwidth = findmaxval(4)   !  RiverData has depth in column 4
   maxflow = 0.0
   minflow = 1.0e6
   maxvel = 0.0
   minvel = 1.0e6
! put depth, width, flow, velocity data in arrays for plotting
   do j = 1, ProfilePoints
     xDepth(j) = sngl(FlowVolumes(1,j))
     yDepth1(j) = 0.0
     yDepth2(j) = sngl(-1.0 * FlowVolumes(3,j))
     yWidth1(j) = -0.5 * FlowVolumes(4,j)
     yWidth2(j) = 0.5 * FlowVolumes(4,j)
     yFlow(j) = sngl(FlowVolumes(2,j))
     yVelocity(j) = yFlow(j)/(35.3*60.0*-1.0*yDepth2(j)*FlowVolumes(4,j))
     if (maxflow .lt. yFlow(j)) maxflow = yFlow(j)
     if (minflow .gt. yFlow(j)) minflow = yFlow(j)
     if (maxvel .lt. yVelocity(j)) maxvel = yVelocity(j)
     if (minvel .gt. yVelocity(j)) minvel = yVelocity(j)
   end do
! put VOC input data in arrays for plotting
! file i/o added 7/30/03 to get VOC Input data for plotting
   open (33, file = 'VOCInputData.dat')
   do j = 1, VOCInputPoints
     xVOCInput(j) = VOCInputs(1,j)
     yVOCInput(j) = VOCInputs(2,j)
     write (33, '(2e15.5)') xVOCInput(j), yVOCInput(j)
   end do
   close (33)
! find log of VOC input maximum and minimum
   vocmin = 100.0
   vocmax = -100.0
   do i = 1, splinepnts
     if (spl_VOCInputs(2,i) .gt. 0.0) then
       if (vocmin .gt. sngl(dlog10(spl_VOCInputs(2,i)))) &
             vocmin = sngl(dlog10(spl_VOCInputs(2,i)))
       if (vocmax .lt. sngl(dlog10(spl_VOCInputs(2,i)))) &
             vocmax = sngl(dlog10(spl_VOCInputs(2,i)))
     endif
   end do
   vocmin = float(int(vocmin)-2)
   vocmax = float(int(vocmax)+1)
! set yVOCInput to hold log(VOC Input data) set zeros to VOCMIN for plotting
   do j = 1, VOCInputPoints
     if (yVOCInput(j) .gt. 0.0) then
       yVOCInput(j) = log10(yVOCInput(j))
     else
       yVOCInput(j) = vocmin
     endif
   end do
! open up the window with the river profile
   if (.not. ProfileWindowOpen) then
     profilewindow%flags  = SysMenuOn + MinButton + MaxButton
     profilewindow%x      = 20
     profilewindow%y      = 20
     profilewindow%width  = 800
     profilewindow%height = 650
     profilewindow%title  = 'Graphical Plots of River Profile Data'
     call WindowOpenChild(ProfileWindow, ProfileWinUnit)
     if (ProfileWinUnit .eq. -1) then
       msg0 = 'Could not open window for display of river profile'
```

```
      msg1 = 'Window Error'
      call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
      call WindowSelect(0)
      call WBitmapPut(MainWinBitmap, 0, 0)
      if (ErrorWindow) then
        call WindowSelect(ErrWinUnit)
        call WBitmapPut(ErrWinBitmap, 0, 0)
      endif
      return
    endif
    ProfileWindowOpen = .true.
  endif
  if (focusprofile .eq. 1) then
    call WindowRaise(ProfileWinUnit)
  elseif (focusprofile .eq. 2) then
    call WindowSelect(ProfileWinUnit)
    focusprofile = 0
  endif
! this is the depth profile plot
  ymin = (-1.0 * MaxDepth - 0.05 * maxdepth)
  ymax = 0.05
  call PlotProfile(xwindowleft, xwindowright, ylast-deltaywindow, ylast, &
                   deltaywindow, xmin, xmax, ymin, ymax, xDepth, yDepth1, &
                   yDepth2, ProfilePoints, 2, 159, 'Distance (km)', &
                   '   Depth-m')
! 159 is bright blue, see col256 in wint/demos
! now plot the width profile
  ylast = ylast - deltaywindow
  ymin = -0.5*MaxWidth - 0.05*Maxwidth
  ymax = 0.5*MaxWidth + 0.05*MaxWidth
  call PlotProfile(xwindowleft, xwindowright, ylast-deltaywindow, ylast, &
       deltaywindow, xmin, xmax, ymin, ymax, xDepth, yWidth1, yWidth2, &
       ProfilePoints, 2, 95, 'Distance (km)', '  Width-m')
! now plot the flow volumes
  ylast = ylast - deltaywindow
  ymin = MinFlow - 0.05 * MinFlow
  ymax = MaxFlow + 0.05 * MaxFlow
  call PlotProfile(xwindowleft, xwindowright, ylast-deltaywindow, ylast,&
deltaywindow, xmin, xmax, ymin, ymax, xDepth, yFlow, &
yFlow, ProfilePoints, 1, 191, 'Distance (km)', &
' Q-m3/s')
! 191 is bright magenta, see col256 in wint/demos
! now plot the velocities
  ylast = ylast - deltaywindow
  ymin = MinVel - 0.05 * MinVel
  ymax = MaxVel + 0.05 * MaxVel
  call PlotProfile(xwindowleft, xwindowright, ylast-deltaywindow, ylast,&
                   deltaywindow, xmin, xmax, ymin, ymax, xDepth, &
                   yVelocity, yVelocity, ProfilePoints, 1, 31, &
                   'Distance (km)', '  Veloc.-m/s')
! 31 is bright red, see col256 in wint/demos
! now plot the VOC input series
  ylast = ylast - deltaywindow
  call PlotProfile(xwindowleft, xwindowright, ylast-deltaywindow, ylast, &
                   deltaywindow, xmin, xmax, vocmin, vocmax, xVOCInput, &
                   yVOCInput, yVOCInput, VOCInputPoints, 1, 127, &
                   'Distance (km)', ' VOC-mol/km')
!  now we can deallocate all the data arrays
  deallocate (xDepth, yDepth1, yDepth2, yWidth1, yWidth2, yFlow, &
              yVelocity, xVOCinput, yVOCInput)
  focusoutput = 1
  focusconcfracoutput = 1
!  this next line will cause the profile window to be brought to the top with each call from the
! main menu.  If you want it to stay in the background with each menu call, set FOCUSPROFILE = 2
  focusprofile = 1
  return
end subroutine ViewRiverProfile
```

```fortran
subroutine VOC_Params (bool_in)
  use msflib
  use winteracter
  use voccom
  implicit none
  INCLUDE 'RESOURCE.FD'
  logical lret, err, bool_in
  integer iret, ierr, iloop
  call unusedqq(bool_in)
  ierr = 0
  msg0 = ''
  msg1 = ''
  if (MenuActive) then
    msg0 = 'Please close open set-up menu\nbefore opening new window'C
    msg1 = 'Window Error'
    call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
    call WindowSelect(0)
    call WBitmapPut(MainWinBitmap, 0, 0)
    if (ErrorWindow) then
      call WindowSelect(ErrWinUnit)
      call WBitmapPut(ErrWinBitmap, 0, 0)
    endif
    if (ProfileWindowOpen) then
      focusprofile = 2
      call ViewRiverProfile(lret)
    endif
    return
  endif
  err = .true.
  menuactive = .true.
! initialize the dialog box
  call WDialogLoad(IDD_VOCParams)
! write the current molecular weight into the dialog box edit field
! write the current init. concentration into the dialog box edit field
! write the current atmos. concentration into the dialog box edit field
  write(err_str(1),'(f9.3)') MolWeight
  write(err_str(2),'(f8.3)') AtmVOCConc
  write(err_str(3),'(e12.4)') Diffusivity
  write(err_str(4),'(e12.4)') Solubility
  write(err_str(5),'(e12.4)') DegradationRate
  call WDialogPutString(IDC_MolWeight, err_str(1))
  call WDialogPutString(IDC_AtmosConc, err_str(2))
  call WDialogPutString(IDC_Diffusivity, err_str(3))
  call WDialogPutString(IDC_Solubility, err_str(4))
  call WDialogPutString(IDC_DegradationRate, err_str(5))
! bring up the dialog box
  call WDialogShow(-1, -1, 0, 2)
  return
end subroutine VOC_Params

subroutine vocdrv
  use dfmt
  use msflib
  use winteracter
  use voccom
  use cfunccom
  implicit none
  include 'resource.fd'
  type(win_message) message
  logical lret
  integer i, j, k, irelab, ifail, iret, numpts, ierr, outputstep, iweir
  real*8 conc(:), work(:,:), sumconcfrac(:)
! conc(num_eqs), work(num_eqs, 20)
  allocatable conc, work, sumconcfrac
  real*8 time_beg, time_end, total_time, clast, convunits, degc, tol, &
         tm, tm0, tm1, &
         gasexchange, degradation, flowconv, concsave, xbeg
```

```
! real*8 external functions
  real*8 cfunc_net, cfunc_comp, dqdt, mass_input, kl_func, kd_func, cs_func
! integer external funtions
  integer mass_source
  external cfunc_net, cfunc_comp, dqdt, mass_input, kl_func, kd_func, &
           cs_func, mass_source, xyplot, xyplot2
! arrays used for plotting data
  real*4 plotarray(2,2,2), plotarray2(:,:,:), total_fraction
  allocatable plotarray2
! allocate array used to hold individ concs from each src and reset to zero
!  SourceNumber one greater than number of actual sources.
!  Extra source is for gas exchange
!  allocate(sourceconc(SourceNumber+1))
!  allocate(sourceconc0(SourceNumber+1))
  allocate(plotarray2(2,2,SourceNumber+1))
  num_eqs = sourcenumber + 3  ! one eq for each src and flow and total conc.
  allocate(conc(num_eqs), work(num_eqs,20), sumconcfrac(num_eqs-3))
  outputstep = 2
  if (WeirNum .gt. 0) then
    iweir = 1   ! start out with the first weir
  else
    iweir = 0
  endif
!  clear out OldData array
  do i = 1, 2
    do j = 1, splinepnts
      do k = 1, 2
        OldData(i,j,k) = 0.0e0
      enddo
    enddo
  enddo
! graphics reinitialization
  PlotInit = .false.      ! reset PlotInit so that axes will be redrawn
  PlotInit2 = .false.     ! reset PlotInit2 so that axes will be redrawn
! set a constant for conversion of concentrations
  convunits = 1.0d3*molweight     ! converts moles/m^3 to ug/L
  if (FlowUnits .eq. 0) then
    flowconv = 1.0d0
  else
    flowconv = 2118.9              ! change m^3/sec to cfm
  endif
! scale factors used of generating the concentration plots
  MaxConc = log10(sngl(max(RiverData(1,6), cs_func(1)*convunits))) + 0.2e0
  if ((RiverData(1,6) .gt. 0.0d0) .and. (cs_func(1) .gt. 0.0d0)) then
    MinConc = log10(sngl(min(RiverData(1,6), cs_func(1)*convunits))) - 0.2e0
  else
    MinConc = -5.0e0
  endif
  MinLength = 0.0e0
  MaxLength = sngl(RiverLength)
! set the initial variables
  total_time = 0.0d0
  plotarray(1,1,1) = 0.0e0
  plotarray(1,1,2) = 0.0e0
  conc(2) = 1.0d-3 * RiverData(1,6) / molweight ! 0.001  ug/L to mol/m^3
  if (conc(2) .gt. 0.0d0) then
    plotarray(2,1,1) = log10(sngl(conc(2) * convunits))
  elseif (cs_func(1) .gt. 0.0e0) then
    plotarray(2,1,1) = log10(sngl(cs_func(1) * convunits))
  else
    plotarray(2,1,1) = -5.0e0
  endif
  if (cs_func(1) .gt. 0.0d0) then
    plotarray(2,1,2) = log10(sngl(cs_func(1) * convunits))
  else
    plotarray(2,1,2) = -5.0e0
  endif
```

```
!  now set up the initial source fractions, src 1=1.0d0, all others=0.0d0
  conc(3) = 1.0d0    ! conc(3) is fraction of source 1
  do i = 4, num_eqs
    conc(i) = 0.0d0
  end do
!  setup the initial values in OldData
  OldPoints = 0
! Now set up the arrays for plotting concentration fractions
  plotarray2(2,1,1) = 1.0e0
  do i = 2, SourceNumber+1
    plotarray2(2,1,i) = 0.0e0
  end do
  do i = 1, SourceNumber+1
    plotarray2(1,1,i) = 0.0e0
  end do
! If saving the data write out the header to the file
  if (DatOut) then
    if (FlowUnits .eq. 0) then
      write (DatFilUnit,'(a\)') '%Dist(km)        C(ug/L)      Flow(m3/s)    V(m/s)      kL(m/s)
VOCInput(mol)    cs(ug/L)    CurrSrc    Initial'
    else
      write (DatFilUnit,'(a\)') '%Dist(km)        C(ug/L)      Flow(cfm)     V(m/s)      kL(m/s)
VOCInput(mol)    cs(ug/L)    CurrSrc    Initial'
    endif
    do j = 1, SourceNumber
      write (datfilunit,'(4x,i2,a\)',iostat=ierr) j, '-Src'
    end do
    do k = 2, SourceNumber
      write (datfilunit,'(1x,i2,a\)',iostat=ierr) k, '-SumSrc'
    end do
    write (datfilunit,'(4x,a)',iostat=ierr) 'Sum-Air'
!   now write the initial data point
    do j = 1, num_eqs-3
      sumconcfrac(j) = 0.0d0
      do k = j+3, 4, -1
        sumconcfrac(j) = sumconcfrac(j) + conc(k)
      end do
    end do
    tm = 0.0d0
    cs = cs_func(1)     ! saturation concentration, f(T, Patm)  (moles/m^3)
    write (datfilunit,'(f12.6,6e13.4,i12,f10.4\)',iostat=ierr) &
      spl_xval(1), conc(2)*convunits, spl_flow(1)*flowconv, spl_veloc(2,1), &
      kl_func(1), tm, cs*convunits, currentsource, conc(3)
    do j = 4, Num_Eqs
      write (datfilunit,'(f10.4\)',iostat=ierr) conc(j)
    end do
    do k = 1, Num_Eqs-4
      write (datfilunit,'(f10.4\)',iostat=ierr) sumconcfrac(k)
    end do
    write (datfilunit,'(f10.4)',iostat=ierr) sumconcfrac(Num_Eqs-3)
  endif
!  begin master loop through the NUMPTS segments of river discretization
    do i = 2,  splinepnts
      time_beg = total_time
      time_end = total_time + spl_timestep(i-1)
      total_time = total_time + spl_timestep(i-1)
      conc(1) = spl_flow(i-1)
!      set values of physico-chemical parameters for use in CFUNC
!      these are passed as parameters in MODULE CFUNCCOM
      kl = kl_func(i-1)    ! gas transfer velocity, f(v, d, w)  (m/s)
      kd = kd_func(i-1)    !  biochemical degradation rate, f(T) (1/s)
      cs = cs_func(i-1)    ! saturation concentration, f(T, Patm)(moles/m^3)
      v = spl_veloc(2,i-1)  ! river velocity (m/s)
      qprime = dqdt(i-1)   ! change in flow with time (m^3/s^2)
!      total VOC input from confluences and
!      distributed sources (moles/sec-sec)
      ii = mass_input(i-1)
```

```
      currentsource = mass_source(i-1)
      j = currentsource
      tm = ii * (time_end - time_beg)
      depth = spl_depth(i-1)
!     set values of parameters needed by D02BAF
      ifail = 0
      tol = tolerance
!     note that TOLERANCE is set by user in dialog menu RUNTIME Parameters
      if ((iweir .gt. 0) .and. (iweir .le. WeirNum)) then
        concsave = conc(2)
        if (WeirPoints(iweir,1) .le. spl_xval(i)) then
          ! the previous segment had a weir
          ! adjust starting concentration to account for aeration by weir
          ! WeirEffic calculated in CalcFlowProfile using WeirEffic
          ! subrotuine in physicochem
          select case (WeirFlow)
            case (0)   ! no flow under weir/dam
              !adjust concentration
              WeirFrac = 1.0d0
              conc(2) = WeirEffic(iweir) * (cs - conc(2)) + conc(2)
            case (1)   ! flow under weir or dam predicted by Darcy's Law
              ! adjust concentration assuming 80% of total flow goes over
              ! weir, 20% goes under
              ! frac come from Darcy's Law assuming K=3000 ft/day (gravel)
              WeirFrac = 0.8d0
              conc(2) = &
                (WeirFrac*conc(1)*(WeirEffic(iweir)*(cs-conc(2))+conc(2))+&
                (1-0d0-WeirFrac)*conc(1)*conc(2))/conc(1)
          end select
          select case (ModelFunction)
            case (0)    ! netflux, only need to change alpha's if Cs > Cb
              if (cs .gt. concsave) then
                do j = 3, num_eqs-1
                  conc(j) = (conc(j)*concsave)/conc(2) !adjust conc fracs
                end do
                conc(num_eqs) = &
                    (conc(num_eqs)*concsave + (conc(2)-concsave))/conc(2)
                !   adjust air fraction
              endif
            case (1)  !component fluxes, see page 134 for discussion
              testsum = 0.0d0
              do j = 3, num_eqs-1
                !adjust concentration fractions for the sources
                conc(j) = &
                    conc(j)*concsave*(1-WeirFrac*WeirEffic(iweir))/conc(2)
                testsum = testsum + conc(j)
              end do
              !adjust air fraction
              conc(num_eqs) = &
                (conc(num_eqs)*concsave*(1-WeirFrac*WeirEffic(iweir)) + &
                 WeirFrac*WeirEffic(iweir)*cs) / conc(2)
              testsum = testsum + conc(num_eqs)
          end select
          iweir = iweir + 1
          ! increment iweir so that next time we don't do it again
        endif
      endif
      tm0 = conc(1) * conc(2)
!     decide which version of CONC to use, NET_FLUX or COMPONENT_FLUX
      select case (ModelFunction)
        case (0)    ! this is for NET FLUX Calculations
          call d02baf(time_beg, time_end, num_eqs, conc, tol, &
                cfunc_net, work, ifail)
        case (1)    ! this is for COMPONENT FLUX Calculations
          call d02baf(time_beg, time_end, num_eqs, conc, tol, &
                cfunc_comp, work, ifail)
        case default  ! defaults to NET FLUX
```

```
          call d02baf(time_beg, time_end, num_eqs, conc, tol, &
               cfunc_net, work, ifail)
        end select
        if (ifail .eq. 3) then
!         IFAIL = 3 means tol is too small, try once with larger value
          tol = 10.0 * tol
          select case (ModelFunction)
            case (0)    ! this is for NET FLUX Calculations
              call d02baf(time_beg, time_end, num_eqs, conc, tol, &
                   cfunc_net, work, ifail)
            case (1)    ! this is for COMPONENT FLUX Calculations
              call d02baf(time_beg, time_end, num_eqs, conc, tol, &
                   cfunc_comp, work, ifail)
            case default  ! defaults to NET FLUX
              call d02baf(time_beg, time_end, num_eqs, conc, tol, &
                   cfunc_net, work, ifail)
          end select
        endif
        if (ifail .ne. 0) then
!           close(22)
          call WindowFontColour(TextBlack, TextWhiteBold)
          msg1 = 'Model Status:  Run halted on error'
          call WindowOutString(0, 1600, msg1)
          lrunning = .FALSE.
          menuactive = .false.
          if (DatOut) then
            close (DatFilUnit)
            DatOut = .false.
            msg0 = 'Closed Output File: '//trim(datfile_out)
            call WindowOutString(0, 1300, msg0)
          endif
!         save final screen into the bitmap for updating
          call WBitmapGet(MainWinBitmap,0)
!          deallocate(sourceconc)
!          deallocate(sourceconc0)
          deallocate(conc)
          deallocate(plotarray2)
          write (msg0, '(a, i2, a)') 'ifail = ', ifail, &
             '  Halt model and check parameters'
          msg1 = 'Error in D02BAF'
          call wmessagebox (OKOnly, ExclamationIcon, CommonOK, msg0, msg1)
          call WindowSelect(0)
          call WBitmapPut(MainWinBitmap, 0, 0)
          if (ErrorWindow) then
            call WindowSelect(ErrWinUnit)
            call WBitmapPut(ErrWinBitmap, 0, 0)
          endif
          if (ProfileWindowOpen) then
            focusprofile = 2
            call ViewRiverProfile(lret)
          endif
          call menuset(1)    ! turn all the menus back on
          call exitthread(0)    !exit code is 0
        endif
!        put new values into OldData
        OldPoints = OldPoints + 1
        OldData(1,OldPoints,1) = sngl(spl_xval(i-1))
        OldData(1,OldPoints,2) = sngl(spl_xval(i-1))
        if (conc(2) .gt. 0.0d0) then
          OldData(2,OldPoints,1) = log10(sngl(conc(2) * convunits))
        else
          OldData(2,OldPoints,1) = -5.0e0
        endif
        if (cs .gt. 0.0d0) then
          OldData(2,OldPoints,2) = log10(sngl(cs * convunits))
        else
          OldData(2,OldPoints,2) = -5.0e0
```

```fortran
        endif
!       Beginning of data plotting routine
        if ((mod(i-1,outputstep) .eq. 0) .and. &
          ((splinepnts - i) .gt. outputstep)) then
         plotarray(1,2,1) = sngl(spl_xval(i+outputstep-1))
         plotarray(1,2,2) = sngl(spl_xval(i+outputstep-1))
         if (conc(2) .gt. 0.0d0) then
           plotarray(2,2,1) = log10(sngl(conc(2) * convunits))
         else
           plotarray(2,2,1) = -5.0e0
         endif
         if (cs_func(i-1) .gt. 0.0d0) then
           plotarray(2,2,2) = log10(sngl(cs_func(i-1) * convunits))
         else
           plotarray(2,2,2) = -5.0e0
         endif
         if ((MaxConc .lt. plotarray(2,2,1)) .or. &
             (MaxConc .lt. plotarray(2,2,2))) then
           PlotInit = .false.
           if (MaxConc .lt. plotarray(2,2,1)) &
             MaxConc = plotarray(2,2,1) + 0.2e0*(MaxConc-MinConc)
           ! conc. in log units,
           if (MaxConc .lt. plotarray(2,2,2)) &
             MaxConc = plotarray(2,2,2) + 0.2e0*(MaxConc-MinConc)
           ! so factor of two increase
         endif
         if ((MinConc .gt. plotarray(2,2,1)) .or. &
             (MinConc .gt. plotarray(2,2,2))) then
           PlotInit = .false.
           if (MinConc .gt. plotarray(2,2,1)) &
             MinConc = plotarray(2,2,1) - 0.2e0*(MaxConc-MinConc)
           ! conc in log units,
           if (MinConc .gt. plotarray(2,2,2)) &
             MinConc = plotarray(2,2,2) - 0.2e0*(MaxConc-MinConc)
           ! so factor of two decrease
         endif
         call xyplot(plotarray)
!        now move new valus of conc frac to old values in plotarray
         do j = 1, 2
           plotarray(1,1,j) = plotarray(1,2,j)
           plotarray(2,1,j) = plotarray(2,2,j)
         end do
!        put the new values into PLOTARRAY2
         total_fraction = 0.0e0
         do j = 1, SourceNumber+1
           plotarray2(1,2,j) = sngl(spl_xval(i+outputstep-1))
           plotarray2(2,2,j) = sngl(conc(j+2))
!          conc(j+2) is source fraction for source j
           total_fraction = total_fraction + plotarray2(2,2,j)
         end do
!      write (22, '(i7, f15.7, e17.7)') i, plotarray2(1,1,1), total_fraction
         call xyplot2(plotarray2, SourceNumber+1)
!        now move new valus of conc frac to old values in plotarray2
         do j = 1, SourceNumber+1
           plotarray2(1,1,j) = plotarray2(1,2,j)
           plotarray2(2,1,j) = plotarray2(2,2,j)
         end do
        endif
!       end of data output if then to plot every outputstepth point
!        write data to file every point if necessary
        if (DatOut) then
          do j = 1, num_eqs-3
            sumconcfrac(j) = 0.0d0
            do k = j+3, 4, -1
              sumconcfrac(j) = sumconcfrac(j) + conc(k)
            end do
          end do
```

```fortran
          write (datfilunit,'(f12.6,6e13.4,i12,f10.4\)',iostat=ierr) &
            spl_xval(i-1), conc(2)*convunits, conc(1)*flowunits, v, kl, &
            tm, cs*convunits, currentsource, conc(3)
          do j = 4, Num_Eqs
            write (datfilunit,'(f10.4\)',iostat=ierr) conc(j)
          end do
          do k = 1, Num_Eqs-4
            write (datfilunit,'(f10.4\)',iostat=ierr) sumconcfrac(k)
          end do
          write (datfilunit,'(f10.4)',iostat=ierr) sumconcfrac(Num_Eqs-3)
        endif
!     check to see if HaltModel has been called
        if (.not. lrunning) then
          msg1 = 'Model Status:  Run halted by user'
          call WindowFontColour(TextRedBold, TextWhiteBold)
          call WindowOutString(0, 1600, msg1)
          call WindowFontColour(TextBlack, TextWhiteBold)
          menuactive = .false.
          if (DatOut) then
            close (DatFilUnit)
            DatOut = .false.
            msg0 = 'Closed Output File: '//trim(datfile_out)
            call WindowOutString(0, 1300, msg0)
          endif
          deallocate(conc, plotarray2)
          call WBitmapGet(MainWinBitmap,0)
!         This is the call that actually terminates the thread
          call menuset(1)    ! turn all the menus back on
          call exitthread(0)     !exit code is 0
        endif
!     end of main do loop over splinepnts
      end do
!   write final data point to file if necessary
    if (DatOut) then
      do j = 1, num_eqs-3
        sumconcfrac(j) = 0.0d0
        do k = j+3, 4, -1
          sumconcfrac(j) = sumconcfrac(j) + conc(k)
        end do
      end do
      write (datfilunit,'(f12.6,6e13.4,i12,f10.4\)',iostat=ierr) &
        spl_xval(splinepnts), conc(2)*convunits, conc(1)*flowunits, v, kl, &
        tm, cs*convunits, currentsource, conc(3)
      do j = 4, Num_Eqs
        write (datfilunit,'(f10.4\)',iostat=ierr) conc(j)
      end do
      do k = 1, Num_Eqs-4
        write (datfilunit,'(f10.4\)',iostat=ierr) sumconcfrac(k)
      end do
      write (datfilunit,'(f10.4)',iostat=ierr) sumconcfrac(Num_Eqs-3)
    endif
!   close(22)
    call WindowFontColour(TextBlack, TextWhiteBold)
    msg1 = 'Model Status:  Run completed'
    call WindowOutString(0, 1600, msg1)
    lrunning = .FALSE.
    menuactive = .false.
    if (DatOut) then
      close (DatFilUnit)
      DatOut = .false.
      msg0 = 'Closed Output File: '//trim(datfile_out)
      call WindowOutString(0, 1300, msg0)
    endif
!   save final screen into the bitmap for updating
    call WBitmapGet(MainWinBitmap,0)
!   deallocate(sourceconc)
!   deallocate(sourceconc0)
```

```
  deallocate(conc)
  deallocate(sumconcfrac)
  deallocate(plotarray2)
  call menuset(1)    ! turn all the menus back on
  call exitthread(0)     !exit code is 0
end subroutine vocdrv

subroutine VOCParam_OK()
  use msflib
  use winteracter
  use voccom
  implicit none
  include 'resource.fd'
  call WDialogUnload()
  menuactive = .false.
  return
end subroutine VOCParam_OK

real*8 function WeirEffic_calc(istruct, q, h, s, Ht)
! parameterizations taken from Gulliver et al. JHE, July 1998, 664-671
!  itype = structure type, 1 = sharp-crested weir (i.e., plunging jet_
!                          2 = ogee-crested weir (spillway, no free jet)
!                          3 = gated sill
!  q = specific discharge = Q/L : Q is flow, L is length (m^2/sec)
!  h = head loss across structure (m)
!  s = submergence of gate lip (only used for type 3) (m)
!  Ht = tailwater depth (m)
use voccom
implicit none
! passed variables
integer istruct
real*8 q, h, s, Ht
!local variables
real*8 nu, tempc, R, F, g, e20, effic, d, ft, fd, fall, do2
! nu = kin visc
! tempc = temperature
! R = reynolds number
! F = Froude number
! g = accel of gravity
! e20 = oxygen transfer coefficient at 20 C
! e = weir efficiency for VOC, returned as WeirEffic
! d = molecular diffusivity of VOC
! ft = temperature correction factor for e20
! fd = diffusivity correction factor for e20
! f = overall correction factor (= ft*fd)
! do2 = diffusivity of oxygen in FW at 20C
! external functions
real*8 diff_calc
external diff_calc
tempc = SurfaceTemp
g = 9.8d0   ! acceleration of gravity
do2 = 1.888d-5   ! in cm^2/sec from scalpha.wb3 workbook
! Kinematic viscosity (nu) in cm^2/sec calc. from temperature in deg-C.
! The underlying data is from data from CRC 63rd edition.
! The polynomial fit was done in the spreadsheet KINVISC.WB1 in QDATA
! The 1.0d-4 factor converts cm^2/sec into m^2/sec
nu = 1.0d-4*(1.7826598d-2 - 5.76464d-4*tempc +  1.12266d-5*tempc**2 - 9.66507d-8*tempc**3)
! Reynolds number
R = q/nu
! Froude number
F = dexp(0.25d0*log(8*g*(h**3)/q**2))  !  (8gh^3/q^2)^1/4
select case (istruct)
  case (1)   !  sharp-crested weir
    e20 = 1.0d0 - (1.0d0/(1+0.24*1.0d-4*(F**1.79)*(R**0.53)))**1.115
  case (2)   !  ogee-crested weir
    e20 = 1.0d0 - dexp(((-0.263d0*h)/(1.0d0+0.215d0*q))-0.203d0*Ht)
  case (3)
```

```
      e20 = 1.0d0 - dexp((-0.0086d0*(h*q/s))-0.118d0)
  case default
    continue
end select
! correction factors taken from Urban et al., October 2001, JHE, 848-859
!temperature correction factor
ft = 1.0d0 + 0.2103d-1*(tempc-2.0d1) + 8.261d-5*(tempc-2.0d1)**2
! diffusivity correction factor
d = diff_calc(tempc, 1)  !  calculate diffusivity of VOC using Wilke-Chang
fd = dsqrt(d/do2)
fall = fd*ft
effic = 1.0d0 - (1.0d0 - e20)**fall
WeirEffic_calc = effic
end function WeirEffic_calc

subroutine xyplot(xyData)
use msflib
use winteracter
use voccom
use cfunccom
implicit none
character*25 dummytitle
character*11 setlabels(2)
data setlabels/'[VOC-total]', '[Atm-Equil]'/
integer  retcode, ipnts, i, j, k
integer  iscale, iticks
real*4 xyData(2,2,2), xData(2), yData1(2), yData2(2), xticks(:), yticks(:), &
       xold(:), yold1(:), yold2(:)
allocatable xticks, yticks, xold, yold1, yold2
parameter (iticks = 5)
if (.not. lrunning) return
allocate (xticks(iticks), yticks(iticks))
ipnts = 2
do i = 1, 2
  xdata(i) = xyData(1,i,1)
  ydata1(i) = xyData(2,i,1)
  ydata2(i) = xyData(2,i,2)
end do
if (.not. Plotinit) then
  call WindowFontColour(NotSet, TextWhite)
  if (xData(1) .eq. 0.0e0) then
    call WindowClearArea(0,1900,9999,9999)   ! reset everything
  else
    call WindowClearArea(0,1900,8499,4999)   ! reset the total conc. plot
  endif
endif
if ((profilewindowopen .or. errorwindow) .and. (focusoutput .eq. 1)) then
  call WindowRaise(0)
  focusoutput = 0
endif
! common calls to set up graphics area for output
! only need to draw the axes once, that is done in the IF-THEN statement
call IGrArea(totalxmin, totalymin, totalxmax, totalymax)
call IGrUnits(minlength, minconc, maxlength, maxconc)
call IPgArea(0.1, 0.15, 0.85, 0.95)
call IPgNewGraph(isets, ipnts, '', '', 'X')
call IPgStyle(1, 0, 0, 0, 191, 191)   ! see col256 in wint/demos color defs
call IPgStyle(2, 0, 0, 0, 159, 159)
call IPgUnits(minlength, minconc, maxlength, maxconc)
! Axis construction, labeling etc. in here
if (.not. PlotInit) then
!  set the x-axis ticks
  call SetTicks(xticks, iticks, minlength, maxlength)
!  set the y-axis ticks
  call SetTicks(yticks, iticks, minconc, maxconc)
  call IGrCharFont(7)
  call IGrCharSize(1.0, 2.0)
```

```
  call IPgXScalePos(0.45)
  call IPgXUserScale(xticks, iticks)
  call IPgYUserScale(yticks, iticks)
  call IPgAxesXY(minlength, minconc)
  call IPgXTickPos(minconc, maxconc)
  call IPgXscale('TN')
  call IPgYscaleLeft('TN')
  call IPgXLabel('Distance (km)','C')
  call IPgYLabelLeft('log[VOC]|ug/L','CV')
  if (xData(1) .gt. 0.0e0) then    ! need to plot OldData
    allocate (xold(oldpoints), yold1(oldpoints), yold2(oldpoints))
    do i = 1, oldpoints
      xold(i) = OldData(1,i,1)
      yold1(i) = OldData(2,i,1)
      yold2(i) = OldData(2,i,2)
    end do
    call IPgNewGraph(isets, oldpoints, '', '', 'X')
    call IPgStyle(1, 0, 0, 0, 191, 191) ! see col256 in wint/demos color defs
    call IPgStyle(2, 0, 0, 0, 159, 159)
    call IPgXYPairs(xold, yold1)
    call IPgXYPairs(xold, yold2)
    deallocate (xold, yold1, yold2)
    call IPgNewGraph(isets, ipnts, '', '', 'X')
    call IPgStyle(1, 0, 0, 0, 191, 191) ! see col256 in wint/demos color defs
    call IPgStyle(2, 0, 0, 0, 159, 159)
  endif
endif
! plot the data
call IPgXYPairs(xData, yData1)
call IPgXYPairs(xData, yData2)
if ((.not. PlotInit) .and. (xData(1) .eq. 0.0e0)) then
  call IPgKeyAll(setlabels,'H')
endif
PlotInit = .true.
deallocate (xticks, yticks)
return
end subroutine xyplot

subroutine xyplot2(xyData, numsets)
use msflib
use dflib
use winteracter
use voccom
use cfunccom
implicit none
character*25 dummytitle
character*8 setlabels(21)
data setlabels/'Src.  1', 'Src.  2', 'Src.  3', 'Src.  4', 'Src.  5', &
               'Src.  6', 'Src.  7', 'Src.  8', 'Src.  9', 'Src. 10', &
               'Src. 11', 'Src. 12', 'Src. 13', 'Src. 14', 'Src. 15', &
               'Src. 16', 'Src. 17', 'Src. 18', 'Src. 19', 'Src. 20', &
               'Src. 21'/
integer  retcode, ipnts, i, j, k, ierr, numsets, iticks
integer  iscale, numpnts
real*4   xyData(2,2,numsets), y11, y12, y21, y22
real*4 xdata(:), ydata(:,:), xticks(:), yticks(:)
allocatable xdata, ydata, xticks, yticks
numpnts = 14      ! changed from 2 for plotting cumulative fractions
if (.not. lrunning) return
setlabels(numsets) = 'Air Src.'
iticks = 5
allocate(xdata(numpnts), ydata(numsets,numpnts))
allocate(xticks(iticks), yticks(iticks))
xdata(1) = xyData(1,1,1)
xdata(2) = xyData(1,2,1)
xdata(3) = xyData(1,2,1)
xdata(4) = xyData(1,1,1)
```

```
xdata(5) = xyData(1,1,1)
xdata(6) = xyData(1,1,1) + 0.111111e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(7) = xyData(1,1,1) + 0.222222e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(8) = xyData(1,1,1) + 0.333333e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(9) = xyData(1,1,1) + 0.444444e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(10) = xyData(1,1,1) + 0.555555e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(11) = xyData(1,1,1) + 0.666666e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(12) = xyData(1,1,1) + 0.777777e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(13) = xyData(1,1,1) + 0.888888e0*(xyData(1,2,1) - xyData(1,1,1))
xdata(14) = xyData(1,2,1)
y11 = 0.0e0
y21 = 0.0e0
do j = 1, numsets
  ydata(j,1) = y11
  ydata(j,2) = y21
  y12 = y11 + xyData(2,1,j)
  y22 = y21 + xyData(2,2,j)
  ydata(j,3) = y22
  ydata(j,4) = y12
  ydata(j,5) = y11
  ydata(j,6) = y12 + 0.111111e0*(y22-y12)
  ydata(j,7) = y11 + 0.222222e0*(y21-y11)
  ydata(j,8) = y12 + 0.333333e0*(y22-y12)
  ydata(j,9) = y11 + 0.444444e0*(y21-y11)
  ydata(j,10) = y12 + 0.555555e0*(y22-y12)
  ydata(j,11) = y11 + 0.666666e0*(y21-y11)
  ydata(j,12) = y12 + 0.777777e0*(y22-y12)
  ydata(j,13) = y11 + 0.888888e0*(y21-y11)
  ydata(j,14) = y22
  y11 = y12
  y21 = y22
end do
if ((profilewindowopen .or. errorwindow) .and. (focusoutput .eq. 1)) then
  call WindowRaise(0)
  focusoutput = 0
endif
! common calls to set up graphics area for output
! only need to draw the axes once, that is done in the IF-THEN statement
call WindowSelect(0)
call IGrArea(totalxmin, fracymin, totalxmax, fracymax)
call IGrUnits(minlength, 0.0e0, maxlength, 1.0e0)
call IPgArea(0.1, 0.15, 0.85, 0.95)
call IPgNewGraph(numsets, numpnts, '', '', 'X')
do i = 1, numsets-1
  call IPgStyle(i, 0, 0, 0, DataSetColor(i), DataSetColor(i))
! see col256 in wint/demos for key to values
end do
call IPgStyle(numsets, 0, 0, 0, 0, 0)    ! Gas Exchange always bright white
call IPgUnits(minlength, 0.0e0, maxlength, 1.0e0)
! Axis construction, labeling etc. in here
if (.not. PlotInit2) then
!  set the x-axis ticks
  call SetTicks(xticks, iticks, minlength, maxlength)
!  set the y-axis ticks
  call SetTicks(yticks, iticks, 0.0e0, 1.0e0)
  call IGrCharFont(7)
  call IGrCharSize(0.75, 1.5)
  call IPgXScalePos(0.45)
  call IPgXUserScale(xticks, iticks)
  call IPgYUserScale(yticks, iticks)
  call IPgAxesXY(minlength, 0.0e0)
  call IPgXTickPos(0.0e0, 1.0e0)
  call IPgXscale('TN')
  call IPgYscaleLeft('TN')
  call IPgXLabel('Distance (km)','C')
  call IPgYLabelLeft('Conc. Fraction','CV')
endif
```

```
! plot the data
do i = 1, numsets
  call IPgXYPairs(xData, yData(i,1:numpnts))
end do
if (.not. PlotInit2) then
  call IPgKeyAll(setlabels,'H')
  PlotInit2 = .true.
endif
write(setlabels(numsets), '(a,i2)') 'Src. ', numsets
deallocate (xdata, ydata, xticks, yticks)
return
end subroutine xyplot2
```

Modules and Compiler Resource Files

```
module voccom
use winteracter
implicit none
!*******************************************************************************
!*   DESCRIPTION FOR MODULE VOCCOM                                            *
!*                                                                            *
!*  This module contains data structures used for the model and windows      *
!*  Before you modify any of these names, make sure you change the names of  *
!*  the corresponding variables in *all* subroutines.  Modify this module    *
!*  carefully.  DO NOT delete items without ensuring that the program        *
!*  will recompile and link                                                  *
!*******************************************************************************
! data definition parameters used below
  integer iaxes, isets, num_eqs
!  parameter (num_eqs=4)
  parameter (iaxes=2, isets=2)
! windows messaging variable
  type(win_message) mainmessage  ! windows messaging var from winteracter
  integer itype    !  type of message
  type (win_style) wc, textwindow, profilewindow, fractionwindow, &
                   errorwindowwc
  integer DataSetColor(21)
  data DataSetColor /223, 31, 159, 191, 127, 95, 63, 110, 78, 207, 162, 237,&
                     46, 64, 128, 192, 32, 223, 31, 159, 191/
  logical PlotInit, PlotOldData, PlotInit2
  character*72 Title, comment(2)
  character*90 ctemp
  character*255 msg0, msg1
! scalar constants used
  real*8 MolWeight, ScVal, HVal, rel_hum, Solubility, Diffusivity, &
      MolarVolume, Density, DegradationRate, wa0, wa1, wa2, wb0, wb1, wb2, &
      salinity, wd0, wd1, wd2, wd3, sola, solb, RiverLength, &
      MaxVelocity, MinVelocity, SurfaceTemp, AirTemp, WindSpeed, &
      AtmosPress, AtmVOCConc, MaxVOCInput, MinVOCInput
  real*8 Tolerance, gasconst
  integer ReachPoints, Reaches, DistributedSources, ProfilePoints, &
      VOCInputPoints, splinepnts, oldpoints, SourceNumber, Boxpnts, &
      WeirNum
  integer diffparam, solparam, savediffparam, savesolparam
  integer DatFilUnit, ParFilUnit
! ModelFuntion flag is used to choose between
!                   NETFLUX and COMPONENTFLUX functions in DE Solver
! WeirFlow flag is used to choose between
!                   flow under weir and no flow under weir
! FlowUnits is used to choose between
!                   m^3/s and cfm in the param files
       integer ModelFunction, WeirFlow, FlowUnits
! single precision constants for Winteracter graphics
  real*4 MaxConc, MinConc, totalxmin, totalxmax, totalymin, totalymax, &
         fracymin, fracymax, minlength, maxlength
! booleans used for program control
```

```fortran
   logical LRunning, DatOut, OpenWindow, MenuActive, ParamFileOK
! Splined array variables used in program.
   real*8  spl_Depth(:), spl_Width(:), spl_Flow(:), spl_xval(:), &
           spl_Timestep(:), spl_Veloc(:,:), spl_VOCInputs(:,:)
   allocatable  spl_Depth, spl_Width, spl_Flow, spl_xval, spl_Timestep, &
               spl_Veloc, spl_VOCInputs
! allocatable array variables used for setting up the splined data.
   real*8  RiverData(:,:), FlowVolumes(:,:), VOCInputs(:,:), WeirPoints(:,:),&
           WeirEffic(:)
   integer WeirType(:)
   allocatable RiverData, FlowVolumes, VOCInputs, WeirPoints, WeirEffic, &
               WeirType
! allocatable array used for plotting data
   real*4 OldData(:,:,:)
   allocatable OldData
! data for constants
   data tolerance /1.0d-8/
   data gasconst /8.20575d-5/      ! R in m3 atm/K mole
   data ParamFileOK /.false./
   data totalxmin, totalxmax, totalymin, totalymax, fracymin, fracymax &
        /0.0e0,    1.0e0,     0.5e0,     0.8e0,     0.0e0,    0.5e0/
   data Boxpnts/400/
! definitions moved to VOCCOM from ERRORCOM for ease of file management
   character*128 err_str(33)
   logical winfunc, ErrorWindow, ProfileWindowOpen, ConcFracWindowOpen, &
           TotalConcWindowOpen
   integer totalconcwinunit, profilewinunit, concfracwinunit, errwinunit, &
           focusprofile, focusoutput, focusconcfracoutput, &
           ErrWinBitmap, MainWinBitmap
   data totalconcwinunit, errwinunit, profilewinunit, concfracwinunit &
        /16, 17, 18, 19/
   data focusoutput, focusconcfracoutput, focusprofile /0, 1, 1/
   data ModelFunction /0/    ! selects NETFLUX version
   data TotalConcWindowOpen, ProfileWindowOpen, ConcFracWindowOpen, &
        ErrorWindow /.false., .false., .false., .false./
! variables involved with the various input files
   character(len=255) parfile_out, parfile_in, datfile_out
   logical Par_File_Read, Par_File_Sav, VOC_File_Sav
   data Par_File_Sav /.true./
   parameter (winfunc = .true.)
   parameter (parfilunit = 14)
   parameter (datfilunit = 15)
END MODULE VOCCOM


module cfunccom
   integer currentsource
   real*8 kl, cs, d, w, v, qprime, ii, kd, depth
!  real*8 sourceconc(:), sourceconc0(:)
!  allocatable sourceconc, sourceconc0
end module cfunccom
//main_win.rc   Note:  specific to Microsoft Developer Studio 6.0
//                     and Compaq Visual Fortran 6.6D
//Microsoft Developer Studio generated resource script.
//
#include "resource.h"

#define APSTUDIO_READONLY_SYMBOLS
/////////////////////////////////////////////////////////////////////////////
//
// Generated from the TEXTINCLUDE 2 resource.
//
#include "afxres.h"

/////////////////////////////////////////////////////////////////////////////
#undef APSTUDIO_READONLY_SYMBOLS
```

```
/////////////////////////////////////////////////////////////////////////
// English (U.S.) resources

#if !defined(AFX_RESOURCE_DLL) || defined(AFX_TARG_ENU)
#ifdef _WIN32
LANGUAGE LANG_ENGLISH, SUBLANG_ENGLISH_US
#pragma code_page(1252)
#endif //_WIN32


/////////////////////////////////////////////////////////////////////////
//
// Dialog
//

IDD_VOCParams DIALOG DISCARDABLE  0, 0, 179, 115
STYLE DS_MODALFRAME | WS_POPUP | WS_CAPTION
CAPTION "VOC Parameters"
FONT 10, "MS Sans Serif"
BEGIN
    DEFPUSHBUTTON   "OK",ID_OKVOCParams,66,97,40,14
    GROUPBOX        "Diffusivity (cm^2/sec)",IDC_STATIC,3,30,81,26
    GROUPBOX        "Solubility (mol/m^3-atm)",IDC_STATIC,92,30,82,26
    GROUPBOX        "Molecular Weight (g/mol)",IDC_STATIC,3,2,81,26
    GROUPBOX        "Degradation Rate (1/sec)",IDC_STATIC,49,62,81,26
    GROUPBOX        "Atmos. Conc. (ppb)",IDC_STATIC,92,2,82,26
    LTEXT           "",IDC_MolWeight,9,13,51,10,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_AtmosConc,100,14,51,10,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_Diffusivity,9,41,51,10,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_Solubility,100,42,51,10,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_DegradationRate,55,74,51,10,SS_SUNKEN | WS_BORDER
END

IDD_EnviroParams DIALOG DISCARDABLE  0, 0, 158, 117
STYLE DS_MODALFRAME | WS_POPUP | WS_CAPTION
CAPTION "Environmental Parameters"
FONT 10, "MS Sans Serif"
BEGIN
    DEFPUSHBUTTON   "OK",ID_OKEnvParams,58,96,40,14
    GROUPBOX        "Atmos. Press. (atm)",IDC_STATIC,78,35,73,24
    GROUPBOX        "Wind Speed (m/s)",IDC_STATIC,7,35,68,24
    GROUPBOX        "Air Temperature (C)",IDC_STATIC,7,6,68,24
    GROUPBOX        "Relative Humidity (%)",IDC_STATIC,42,64,73,24
    LTEXT           "",IDC_AirTemp,16,16,51,9,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_WindSpeed,16,45,51,9,SS_CENTERIMAGE | SS_SUNKEN |
                    WS_BORDER
    LTEXT           "",IDC_AtmPressure,88,45,51,9,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_RelativeHumidity,52,74,51,9,SS_SUNKEN | WS_BORDER
    GROUPBOX        "Water Temperature (C)",IDC_STATIC,78,6,73,24
    LTEXT           "",IDC_WaterTemp,90,16,51,9,SS_CENTERIMAGE | SS_SUNKEN |
                    WS_BORDER
END

IDD_RuntimeParams DIALOG DISCARDABLE  0, 0, 246, 112
STYLE DS_MODALFRAME | WS_POPUP | WS_CAPTION
CAPTION "Runtime Parameters"
FONT 10, "MS Sans Serif"
BEGIN
    DEFPUSHBUTTON   "OK",ID_OKModelParams,96,94,50,14
    LTEXT           "Runge-Kutta Tolerance",IDC_STATIC,2,3,74,8
    LTEXT           "Simulation Title",IDC_STATIC,2,29,50,10
    LTEXT           "Comments",IDC_STATIC,2,55,35,10
    LTEXT           "",IDC_Comment1,2,65,240,12,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_Comment2,2,79,240,12,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_Title,2,40,240,12,SS_SUNKEN | WS_BORDER
    LTEXT           "",IDC_Tolerance,2,14,69,11,SS_SUNKEN | WS_BORDER
    LTEXT           "Number of Boxes per Reach",IDC_STATIC,92,3,85,8
    EDITTEXT        IDC_NumberOfBoxes,92,14,65,12,ES_AUTOHSCROLL
```

```
END

IDD_HydrogParamsList DIALOG DISCARDABLE  0, 0, 349, 159
STYLE DS_MODALFRAME | WS_POPUP | WS_CAPTION | WS_SYSMENU
CAPTION "Hydrological Parameters"
FONT 8, "MS Sans Serif"
BEGIN
    DEFPUSHBUTTON   "OK",ID_HydrogOK,149,138,50,14
    LISTBOX         IDC_HydrogParamLIST,7,49,335,84,LBS_SORT |
                    LBS_USETABSTOPS | LBS_NOINTEGRALHEIGHT | LBS_NOSEL |
                    WS_VSCROLL | WS_TABSTOP
    LTEXT           "No.     Type       Start (km)        End (km)           Z (m)
W (m)              Q(cfm)                 [VOC] (ug/L)    No.",
                    IDC_STATIC,7,40,335,8
    LTEXT           "Reach\nPoint",IDC_STATIC,7,24,22,15
    LTEXT           "Source",IDC_STATIC,310,31,25,7
    LTEXT           "Reach",IDC_STATIC,29,32,22,9
    CTEXT           "River Length: ",IDC_STATIC,7,8,42,8
    CTEXT           "Segments: ",IDC_STATIC,141,8,35,8
    CONTROL         "Distributed Sources:",IDC_STATIC,"Static",
                    SS_LEFTNOWORDWRAP | WS_GROUP,248,8,63,10
    CTEXT           "Static",IDC_TotalLength,49,7,40,10,SS_CENTERIMAGE |
                    SS_SUNKEN | WS_BORDER
    CTEXT           "Static",IDC_ReachPoints,176,7,32,10,SS_CENTERIMAGE |
                    SS_SUNKEN | WS_BORDER
    CTEXT           "Static",IDC_DistributedSourcePoints,313,8,29,10,
                    SS_CENTERIMAGE | SS_SUNKEN | WS_BORDER
END

/////////////////////////////////////////////////////////////////////////
//
// DESIGNINFO
//

#ifdef APSTUDIO_INVOKED
GUIDELINES DESIGNINFO DISCARDABLE
BEGIN
    IDD_VOCParams, DIALOG
    BEGIN
        LEFTMARGIN, 3
        RIGHTMARGIN, 174
        TOPMARGIN, 2
        BOTTOMMARGIN, 111
    END

    IDD_EnviroParams, DIALOG
    BEGIN
        LEFTMARGIN, 7
        RIGHTMARGIN, 151
        TOPMARGIN, 6
        BOTTOMMARGIN, 110
    END

    IDD_RuntimeParams, DIALOG
    BEGIN
        LEFTMARGIN, 2
        RIGHTMARGIN, 242
        TOPMARGIN, 3
        BOTTOMMARGIN, 108
    END

    IDD_HydrogParamsList, DIALOG
    BEGIN
        LEFTMARGIN, 7
        RIGHTMARGIN, 342
        TOPMARGIN, 7
        BOTTOMMARGIN, 152
```

```
    END
END
#endif   // APSTUDIO_INVOKED

#ifdef APSTUDIO_INVOKED
/////////////////////////////////////////////////////////////////////////////
//
// TEXTINCLUDE
//

1 TEXTINCLUDE DISCARDABLE
BEGIN
    "resource.h\0"
END
2 TEXTINCLUDE DISCARDABLE
BEGIN
    "#include ""afxres.h""\r\n"
    "\0"
END
3 TEXTINCLUDE DISCARDABLE
BEGIN
    "\r\n"
    "\0"
END
#endif   // APSTUDIO_INVOKED
/////////////////////////////////////////////////////////////////////////////
//
// Icon
//

// Icon with lowest ID value placed first to ensure application icon
// remains consistent on all systems.
IDI_ICON1              ICON    DISCARDABLE     "icon1.ico"

#ifndef _MAC
/////////////////////////////////////////////////////////////////////////////
//
// Version
//
VS_VERSION_INFO VERSIONINFO
 FILEVERSION 1,0,0,1
 PRODUCTVERSION 1,0,0,1
 FILEFLAGSMASK 0x3fL
#ifdef _DEBUG
 FILEFLAGS 0x1L
#else
 FILEFLAGS 0x0L
#endif
 FILEOS 0x40004L
 FILETYPE 0x1L
 FILESUBTYPE 0x0L
BEGIN
    BLOCK "StringFileInfo"
    BEGIN
        BLOCK "040904b0"
        BEGIN
            VALUE "CompanyName", "APL-UW\0"
            VALUE "FileDescription", "StreamVOC\0"
            VALUE "FileVersion", "1, 0, 0, 1\0"
            VALUE "InternalName", "StreamVOC\0"
            VALUE "LegalCopyright", "Copyright © 2002\0"
            VALUE "OriginalFilename", "streamvoc.exe\0"
            VALUE "ProductName", "StreamVOC\0"
            VALUE "ProductVersion", "1, 0, 0, 1\0"
        END
    END
    BLOCK "VarFileInfo"
```

```
    BEGIN
        VALUE "Translation", 0x409, 1200
    END
END
#endif    // !_MAC

/////////////////////////////////////////////////////////////////////////////
//
// Menu
//

IDR_MENU1 MENU DISCARDABLE
BEGIN
    POPUP "&File "
    BEGIN
        MENUITEM "&Read Parameter File",        IDD_LoadParamFile
        MENUITEM "&Save VOC Model Results",     IDD_SAVERESULTS, GRAYED
        MENUITEM "E&xit",                       IDD_Exit
    END
    POPUP "&View Parameters"
    BEGIN
        MENUITEM "&VOC Parameters",             IDD_ViewVOCParams, GRAYED
        MENUITEM "&Environmental Parameters",   IDD_EnviroParams, GRAYED
        MENUITEM "&Hydrographical Parameters",  IDD_HydrogParams, GRAYED
        MENUITEM "&Runtime Parameters",         IDD_RuntimeParameters
        , GRAYED
        MENUITEM "&Display River Profile",      IDD_ViewProfile, GRAYED
    END
    POPUP "&Run"
    BEGIN
        MENUITEM "&Start Model",                IDD_STARTMODEL, GRAYED
        MENUITEM "&Halt Model",                 IDD_HaltModel, GRAYED
    END
    POPUP "&Help"
    BEGIN
        MENUITEM "&About SteamVOC",             IDD_AboutBox
    END
END

/////////////////////////////////////////////////////////////////////////////
//
// String Table
//

STRINGTABLE DISCARDABLE
BEGIN
    IDS_ParameterFileString "Parameter Files (*.par)|*.par|"
    IDS_DataFileString      "ASCII Data Files(*.dat)|*.dat|ASCII Text Files (*.txt)|*.txt|"
END
#endif    // English (U.S.) resources

/////////////////////////////////////////////////////////////////////////////

#ifndef APSTUDIO_INVOKED

/////////////////////////////////////////////////////////////////////////////
//
// Generated from the TEXTINCLUDE 3 resource.
//
/////////////////////////////////////////////////////////////////////////////

#endif    // not APSTUDIO_INVOKED

// END main_win.rc
```

```
// resource.h header file
//{{NO_DEPENDENCIES}}
// Microsoft Developer Studio generated include file.
// Used by main_win.rc
//
#define IDS_ParameterFileString        1
#define IDS_DataFileString             2
#define IDD_LoadParamFile              101
#define IDD_MTBEParams                 102
#define IDD_VOCParams                  102
#define IDD_MeteorParams               103
#define IDD_EnviroParams               103
#define IDD_TimeSeriesEntry            105
#define IDD_RuntimeParams              110
#define IDD_ResetParams                111
#define IDD_HydrogParams               112
#define IDD_DiffParam                  113
#define IDD_Exit                       113
#define IDD_SolParam                   114
#define IDI_ICON1                      115
#define IDR_MENU1                      124
#define IDD_HydrogParamsList           127
#define IDC_MTBEInputSeries            1014
#define IDC_WindSpeed                  1017
#define IDC_AirTemp                    1018
#define IDC_AtmPressure                1019
#define IDC_WaterTemp                  1020
#define IDC_Tolerance                  1053
#define IDC_Inflow                     1054
#define IDC_OutputDistance             1054
#define IDC_CallDiffParam              1055
#define IDC_MixedLayer                 1061
#define IDC_SurfaceTemp                1062
#define IDC_LakeDepth                  1063
#define IDC_LakeArea                   1064
#define IDC_ReachPointEntry            1064
#define IDC_AtmMTBEConc                1065
#define IDC_DistributedSourceEntry     1065
#define IDC_MolWeight                  1066
#define IDC_InitialConc                1067
#define IDC_Diffusivity                1067
#define IDC_AtmosConc                  1068
#define IDC_DiffButtWilk               1069
#define IDC_Solubility                 1069
#define IDC_DiffButtWann               1070
#define IDC_Wank_a0                    1071
#define IDC_Wank_a1                    1072
#define IDC_Wank_a2                    1073
#define IDC_Wank_a3                    1074
#define IDC_MolarVolume                1075
#define IDC_SolButtWann                1076
#define IDC_Wank_a0_sol                1077
#define IDC_Wank_a1_sol                1078
#define IDC_Wank_a2_sol                1079
#define IDC_Wank_a3_sol                1080
#define IDC_Wank_Salinity              1080
#define IDC_SolButtRobbins             1081
#define IDC_RobbinsA                   1082
#define IDC_RobbinsB                   1083
#define IDC_CallSolParam               1084
#define IDC_Comment1                   1085
#define IDC_DegradationRate            1085
#define IDC_Title                      1087
#define IDC_Comment2                   1088
#define IDC_UOK3                       1089
#define IDC_UMonthly1                  1090
```

```
#define IDC_UWeekly1                      1091
#define IDC_TAOK3                         1092
#define IDC_TAMonthly1                    1093
#define IDC_TAWeekly1                     1094
#define IDC_PAOK3                         1095
#define IDC_PAMonthly1                    1096
#define IDC_PAWeekly1                     1097
#define IDC_TotalTime                     1098
#define IDC_OutputTimestep                1099
#define IDC_ViewRiverProfile              1162
#define IDC_CurrentWorkDir                1163
#define IDC_DataDirectory                 1164
#define IDC_TimeSeriesFilename            1165
#define IDC_FileStatus                    1166
#define IDC_FileStatus2                   1167
#define IDC_LocalTitle                    1185
#define IDC_RiverPhysicalData1            1191
#define IDC_RiverPhysicalData2            1192
#define ID_OKEnvParams                    1192
#define IDC_RiverPhysicalData3            1193
#define IDC_InflowHeightMonthly           1194
#define IDC_ReachPoints1                  1194
#define IDC_TotalLength                   1194
#define IDC_InflowHeightWeekly            1195
#define IDC_RiverPhysicalData4            1195
#define IDC_InflowHeightDaily             1196
#define IDC_RiverPhysicalData5            1196
#define IDC_InflowHeightOK                1197
#define IDC_RiverPhysicalData6            1197
#define IDC_InflowHeightOK2               1198
#define IDC_RiverPhysicalData7            1198
#define IDC_InflowHeightWeekly1           1199
#define IDC_RiverPhysicalData8            1199
#define IDC_InflowHeightMonthly1          1200
#define IDC_RiverPhysicalData9            1200
#define IDC_InflowHeightOK3               1201
#define IDC_RiverPhysicalData10           1201
#define IDC_OutflowHeightWeekly1          1202
#define IDC_RiverPhysicalData11           1202
#define IDC_OutflowHeightMonthly1         1203
#define IDC_RiverPhysicalData12           1203
#define IDC_OutflowHeightOK3              1204
#define IDC_RiverPhysicalData13           1204
#define IDC_RiverPhysicalData14           1205
#define IDC_OutflowHeightOK2              1206
#define IDC_RiverPhysicalData15           1206
#define IDC_EpiLossRate                   1207
#define IDC_RiverPhysicalData16           1207
#define IDC_EpiLossWeekly1                1208
#define IDC_RiverPhysicalData17           1208
#define IDC_EpiLossMonthly1               1209
#define IDC_RiverPhysicalData18           1209
#define IDC_EpiLossOK3                    1210
#define IDC_RiverPhysicalData19           1210
#define IDC_HypLossRate                   1211
#define IDC_RiverPhysicalData20           1211
#define IDC_HypLossOK3                    1212
#define IDC_DistributedSourceData1        1212
#define ID_OKHydroParams                  1212
#define IDC_HypLossMonthly1               1213
#define IDC_DistributedSourceData2        1213
#define ID_OKModelParams                  1213
#define IDC_HypLossWeekly1                1214
#define IDC_DistributedSourceData3        1214
#define ID_OKVOCParams                    1214
#define IDC_EpiLossMonthly                1215
#define IDC_DistributedSourceData4        1215
```

```
#define IDC_NumberOfBoxes                 1215
#define IDC_EpiLossWeekly                 1216
#define IDC_DistributedSourceData5        1216
#define IDC_EpiLossDaily                  1217
#define IDC_DistributedSourceData6        1217
#define IDC_EpiLossOK2                    1218
#define IDC_DistributedSourceData7        1218
#define IDC_EpiLossOK                     1219
#define IDC_DistributedSourceData8        1219
#define IDC_HypLossMonthly               1220
#define IDC_DistributedSourceData9        1220
#define IDC_HypLossWeekly                 1221
#define IDC_DistributedSourceData10       1221
#define IDC_HypLossDaily                  1222
#define IDC_DistributedSourcePoints2      1222
#define IDC_ReachPoints                   1222
#define IDC_HypLossOK2                    1223
#define IDC_DistributedSourcePoints3      1223
#define IDC_DistributedSourcePoints       1223
#define IDC_HypLossOK                     1224
#define IDC_HydrogParamLIST               1224
#define IDC_Wank_b0_sol                   1225
#define ID_HydrogOK                       1225
#define IDC_Wank_b1_sol                   1226
#define IDC_Wank_b2_sol                   1227
#define IDC_DataUnits                     1228
#define IDC_MonthlyTitle                  1229
#define IDC_GraphData                     1232
#define IDC_LoadData                      1233
#define IDC_RDErrorMessage                1235
#define IDC_ScDay                         1236
#define IDC_ScVal                         1237
#define IDC_CalcSc                        1238
#define IDC_HDay                          1239
#define IDC_HVal                          1240
#define IDC_CalcH                         1241
#define IDC_RelativeHumidity              1242
#define IDD_STARTMODEL                    40004
#define IDD_HaltModel                     40005
#define IDD_ViewVOCParams                 40006
#define IDD_SAVERESULTS                   40007
#define IDD_RuntimeParameters             40008
#define IDD_ViewProfile                   40009
#define IDD_AboutBox                      40010
// Next default values for new objects
//
#ifdef APSTUDIO_INVOKED
#ifndef APSTUDIO_READONLY_SYMBOLS
#define _APS_NEXT_RESOURCE_VALUE          128
#define _APS_NEXT_COMMAND_VALUE           40011
#define _APS_NEXT_CONTROL_VALUE           1226
#define _APS_NEXT_SYMED_VALUE             101
#endif
#endif
//end resource.h


// resource.fd
!MS$FREEFORM
! Microsoft Developer Studio generated include file.
! Used by main_win.rc
!
      integer, parameter :: IDS_ParameterFileString      = 1
      integer, parameter :: IDS_DataFileString           = 2
      integer, parameter :: IDD_LoadParamFile            = 101
      integer, parameter :: IDD_MTBEParams               = 102
      integer, parameter :: IDD_VOCParams                = 102
```

```
integer, parameter :: IDD_MeteorParams               = 103
integer, parameter :: IDD_EnviroParams               = 103
integer, parameter :: IDD_TimeSeriesEntry            = 105
integer, parameter :: IDD_RuntimeParams              = 110
integer, parameter :: IDD_ResetParams                = 111
integer, parameter :: IDD_HydrogParams               = 112
integer, parameter :: IDD_DiffParam                  = 113
integer, parameter :: IDD_Exit                       = 113
integer, parameter :: IDD_SolParam                   = 114
integer, parameter :: IDI_ICON1                      = 115
integer, parameter :: IDR_MENU1                      = 124
integer, parameter :: IDD_HydrogParamsList           = 127
integer, parameter :: IDC_MTBEInputSeries            = 1014
integer, parameter :: IDC_WindSpeed                  = 1017
integer, parameter :: IDC_AirTemp                    = 1018
integer, parameter :: IDC_AtmPressure                = 1019
integer, parameter :: IDC_WaterTemp                  = 1020
integer, parameter :: IDC_Tolerance                  = 1053
integer, parameter :: IDC_Inflow                     = 1054
integer, parameter :: IDC_OutputDistance             = 1054
integer, parameter :: IDC_CallDiffParam              = 1055
integer, parameter :: IDC_MixedLayer                 = 1061
integer, parameter :: IDC_SurfaceTemp                = 1062
integer, parameter :: IDC_LakeDepth                  = 1063
integer, parameter :: IDC_LakeArea                   = 1064
integer, parameter :: IDC_ReachPointEntry            = 1064
integer, parameter :: IDC_AtmMTBEConc                = 1065
integer, parameter :: IDC_DistributedSourceEntry     = 1065
integer, parameter :: IDC_MolWeight                  = 1066
integer, parameter :: IDC_InitialConc                = 1067
integer, parameter :: IDC_Diffusivity                = 1067
integer, parameter :: IDC_AtmosConc                  = 1068
integer, parameter :: IDC_DiffButtWilk               = 1069
integer, parameter :: IDC_Solubility                 = 1069
integer, parameter :: IDC_DiffButtWann               = 1070
integer, parameter :: IDC_Wank_a0                    = 1071
integer, parameter :: IDC_Wank_a1                    = 1072
integer, parameter :: IDC_Wank_a2                    = 1073
integer, parameter :: IDC_Wank_a3                    = 1074
integer, parameter :: IDC_MolarVolume                = 1075
integer, parameter :: IDC_SolButtWann                = 1076
integer, parameter :: IDC_Wank_a0_sol                = 1077
integer, parameter :: IDC_Wank_a1_sol                = 1078
integer, parameter :: IDC_Wank_a2_sol                = 1079
integer, parameter :: IDC_Wank_a3_sol                = 1080
integer, parameter :: IDC_Wank_Salinity              = 1080
integer, parameter :: IDC_SolButtRobbins             = 1081
integer, parameter :: IDC_RobbinsA                   = 1082
integer, parameter :: IDC_RobbinsB                   = 1083
integer, parameter :: IDC_CallSolParam               = 1084
integer, parameter :: IDC_Comment1                   = 1085
integer, parameter :: IDC_DegradationRate            = 1085
integer, parameter :: IDC_Title                      = 1087
integer, parameter :: IDC_Comment2                   = 1088
integer, parameter :: IDC_UOK3                       = 1089
integer, parameter :: IDC_UMonthly1                  = 1090
integer, parameter :: IDC_UWeekly1                   = 1091
integer, parameter :: IDC_TAOK3                      = 1092
integer, parameter :: IDC_TAMonthly1                 = 1093
integer, parameter :: IDC_TAWeekly1                  = 1094
integer, parameter :: IDC_PAOK3                      = 1095
integer, parameter :: IDC_PAMonthly1                 = 1096
integer, parameter :: IDC_PAWeekly1                  = 1097
integer, parameter :: IDC_TotalTime                  = 1098
integer, parameter :: IDC_OutputTimestep             = 1099
integer, parameter :: IDC_ViewRiverProfile           = 1162
integer, parameter :: IDC_CurrentWorkDir             = 1163
```

```
integer, parameter :: IDC_DataDirectory          = 1164
integer, parameter :: IDC_TimeSeriesFilename      = 1165
integer, parameter :: IDC_FileStatus              = 1166
integer, parameter :: IDC_FileStatus2             = 1167
integer, parameter :: IDC_LocalTitle              = 1185
integer, parameter :: IDC_RiverPhysicalData1      = 1191
integer, parameter :: IDC_RiverPhysicalData2      = 1192
integer, parameter :: ID_OKEnvParams              = 1192
integer, parameter :: IDC_RiverPhysicalData3      = 1193
integer, parameter :: IDC_InflowHeightMonthly     = 1194
integer, parameter :: IDC_ReachPoints1            = 1194
integer, parameter :: IDC_TotalLength             = 1194
integer, parameter :: IDC_InflowHeightWeekly      = 1195
integer, parameter :: IDC_RiverPhysicalData4      = 1195
integer, parameter :: IDC_InflowHeightDaily       = 1196
integer, parameter :: IDC_RiverPhysicalData5      = 1196
integer, parameter :: IDC_InflowHeightOK          = 1197
integer, parameter :: IDC_RiverPhysicalData6      = 1197
integer, parameter :: IDC_InflowHeightOK2         = 1198
integer, parameter :: IDC_RiverPhysicalData7      = 1198
integer, parameter :: IDC_InflowHeightWeekly1     = 1199
integer, parameter :: IDC_RiverPhysicalData8      = 1199
integer, parameter :: IDC_InflowHeightMonthly1    = 1200
integer, parameter :: IDC_RiverPhysicalData9      = 1200
integer, parameter :: IDC_InflowHeightOK3         = 1201
integer, parameter :: IDC_RiverPhysicalData10     = 1201
integer, parameter :: IDC_OutflowHeightWeekly1    = 1202
integer, parameter :: IDC_RiverPhysicalData11     = 1202
integer, parameter :: IDC_OutflowHeightMonthly1   = 1203
integer, parameter :: IDC_RiverPhysicalData12     = 1203
integer, parameter :: IDC_OutflowHeightOK3        = 1204
integer, parameter :: IDC_RiverPhysicalData13     = 1204
integer, parameter :: IDC_RiverPhysicalData14     = 1205
integer, parameter :: IDC_OutflowHeightOK2        = 1206
integer, parameter :: IDC_RiverPhysicalData15     = 1206
integer, parameter :: IDC_EpiLossRate             = 1207
integer, parameter :: IDC_RiverPhysicalData16     = 1207
integer, parameter :: IDC_EpiLossWeekly1          = 1208
integer, parameter :: IDC_RiverPhysicalData17     = 1208
integer, parameter :: IDC_EpiLossMonthly1         = 1209
integer, parameter :: IDC_RiverPhysicalData18     = 1209
integer, parameter :: IDC_EpiLossOK3              = 1210
integer, parameter :: IDC_RiverPhysicalData19     = 1210
integer, parameter :: IDC_HypLossRate             = 1211
integer, parameter :: IDC_RiverPhysicalData20     = 1211
integer, parameter :: IDC_HypLossOK3              = 1212
integer, parameter :: IDC_DistributedSourceData1  = 1212
integer, parameter :: ID_OKHydroParams            = 1212
integer, parameter :: IDC_HypLossMonthly1         = 1213
integer, parameter :: IDC_DistributedSourceData2  = 1213
integer, parameter :: ID_OKModelParams            = 1213
integer, parameter :: IDC_HypLossWeekly1          = 1214
integer, parameter :: IDC_DistributedSourceData3  = 1214
integer, parameter :: ID_OKVOCParams              = 1214
integer, parameter :: IDC_EpiLossMonthly          = 1215
integer, parameter :: IDC_DistributedSourceData4  = 1215
integer, parameter :: IDC_NumberOfBoxes           = 1215
integer, parameter :: IDC_EpiLossWeekly           = 1216
integer, parameter :: IDC_DistributedSourceData5  = 1216
integer, parameter :: IDC_EpiLossDaily            = 1217
integer, parameter :: IDC_DistributedSourceData6  = 1217
integer, parameter :: IDC_EpiLossOK2              = 1218
integer, parameter :: IDC_DistributedSourceData7  = 1218
integer, parameter :: IDC_EpiLossOK               = 1219
integer, parameter :: IDC_DistributedSourceData8  = 1219
integer, parameter :: IDC_HypLossMonthly          = 1220
integer, parameter :: IDC_DistributedSourceData9  = 1220
```

```
      integer, parameter :: IDC_HypLossWeekly            = 1221
      integer, parameter :: IDC_DistributedSourceData10  = 1221
      integer, parameter :: IDC_HypLossDaily             = 1222
      integer, parameter :: IDC_DistributedSourcePoints2 = 1222
      integer, parameter :: IDC_ReachPoints              = 1222
      integer, parameter :: IDC_HypLossOK2               = 1223
      integer, parameter :: IDC_DistributedSourcePoints3 = 1223
      integer, parameter :: IDC_DistributedSourcePoints  = 1223
      integer, parameter :: IDC_HypLossOK                = 1224
      integer, parameter :: IDC_HydrogParamLIST          = 1224
      integer, parameter :: IDC_Wank_b0_sol              = 1225
      integer, parameter :: ID_HydrogOK                  = 1225
      integer, parameter :: IDC_Wank_b1_sol              = 1226
      integer, parameter :: IDC_Wank_b2_sol              = 1227
      integer, parameter :: IDC_DataUnits                = 1228
      integer, parameter :: IDC_MonthlyTitle             = 1229
      integer, parameter :: IDC_GraphData                = 1232
      integer, parameter :: IDC_LoadData                 = 1233
      integer, parameter :: IDC_RDErrorMessage           = 1235
      integer, parameter :: IDC_ScDay                    = 1236
      integer, parameter :: IDC_ScVal                    = 1237
      integer, parameter :: IDC_CalcSc                   = 1238
      integer, parameter :: IDC_HDay                     = 1239
      integer, parameter :: IDC_HVal                     = 1240
      integer, parameter :: IDC_CalcH                    = 1241
      integer, parameter :: IDC_RelativeHumidity         = 1242
      integer, parameter :: IDD_STARTMODEL               = 40004
      integer, parameter :: IDD_HaltModel                = 40005
      integer, parameter :: IDD_ViewVOCParams            = 40006
      integer, parameter :: IDD_SAVERESULTS              = 40007
      integer, parameter :: IDD_RuntimeParameters        = 40008
      integer, parameter :: IDD_ViewProfile              = 40009
      integer, parameter :: IDD_AboutBox                 = 40010
//end resource.fd
```

Appendix 2. StreamVOC Model Input Parameter Files

2–1. Parameter File for Acetone with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1        0        0
 Total Length of River (km)
        2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m^3/s)    Conc.(ug/L)
 1    0.0          0.0         0.30        5.5         0.354          0.557
 2    0.0          0.096       0.30        5.5         0.037          1.79
 3    0.096        0.096       0.53        7.3         0.0            0.00
 4    0.096        0.400       0.53        7.3         0.023          0.00
 5    0.400        0.400       0.76        7.9         0.0            0.00
 6    0.400        0.540       0.76        7.9         0.093          0.00
 7    0.540        0.540       0.34        22.8        0.0            0.00
 8    0.540        1.09        0.34        22.8        -0.173         0.00
 9    1.09         1.09        0.64        8.5         0.0            0.00
10    1.09         1.15        0.64        8.5         0.054          0.43
11    1.15         1.15        0.79        7.3         0.0            0.00
12    1.15         1.23        0.79        7.3         -0.059         0.00
13    1.23         1.23        0.37        3.6         0.0            0.00
14    1.23         1.647       0.37        3.6         -0.026         0.00
15    1.647        1.647       2.0         100.0       0.202          0.00
16    1.647        1.897       2.0         100.0       0.016          0.00
17    1.897        1.897       2.0         10.0        0.0            0.00
18    1.897        2.147       2.0         10.0        0.0            0.00
19    2.147        2.147       2.0         90.0        0.0            0.00
20    2.147        2.293       2.0         90.0        0.012          0.99
21    2.293        2.293       1.07        10.7        0.0            0.00
22    2.293        2.736       1.07        10.7        0.031          0.61
23    2.736        2.736       0.64        7.9         0.0            0.00
24    2.736        2.811       0.64        7.9         0.051          0.00
25    2.811        2.811       0.64        7.9         0.0            0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.69
 VOC molecular weight in g/mole
       58.08
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
       73.42
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
7.034  5043
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.10;~Aberjona~River~Data;July-11-2001
Acetone~with~7-11-01~groundwater~flows
Groundwater~sources~included~acetone
  Begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#    Location(km)    length    height    silldepth(m)    Tailstockdepth(m)    Type
  1           2.293         10       0.9        0.0              1.07               1
  2           2.740          5       0.5        0.0              0.64               2
\river_model\Aberjona_Data\aberjona_gw_acetone02.dat
```

2–2. Parameter File for Benzene with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)   Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0        0.30        5.5         0.354         0.009
 2    0.0          0.096      0.30        5.5         0.037         0.00
 3    0.096        0.096      0.53        7.3         0.0           0.00
 4    0.096        0.400      0.53        7.3         0.023         0.00
 5    0.400        0.400      0.76        7.9         0.0           0.00
 6    0.400        0.540      0.76        7.9         0.093         0.00
 7    0.540        0.540      0.34        22.8        0.0           0.00
 8    0.540        1.09       0.34        22.8        -0.173        0.00
 9    1.09         1.09       0.64        8.5         0.0           0.00
10    1.09         1.15       0.64        8.5         0.054         0.00
11    1.15         1.15       0.79        7.3         0.0           0.00
12    1.15         1.23       0.79        7.3         -0.059        0.00
13    1.23         1.23       0.37        3.6         0.0           0.00
14    1.23         1.647      0.37        3.6         -0.026        0.00
15    1.647        1.647      2.0         100.0       0.202         0.05
16    1.647        1.897      2.0         100.0       0.016         0.00
17    1.897        1.897      2.0         10.0        0.0           0.00
18    1.897        2.147      2.0         10.0        0.0           0.00
19    2.147        2.147      2.0         90.0        0.0           0.00
20    2.147        2.293      2.0         90.0        0.012         0.00
21    2.293        2.293      1.07        10.7        0.0           0.00
22    2.293        2.736      1.07        10.7        0.031         0.00
23    2.736        2.736      0.64        7.9         0.0           0.00
24    2.736        2.811      0.64        7.9         0.051         0.00
25    2.811        2.811      0.64        7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.20
 VOC molecular weight in g/mole
       78.12
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       94.27
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
       7.924 3918
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
      0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;August-20-2003
Benzene~with~7-11-01~groundwater~flows
Groundwater~sources~included
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#    Location(km)    length   height   silldepth(m)    Tailstockdepth(m)    Type
 1          2.293          10      0.9      0.0             1.07                 1
 2          2.740           5      0.5      0.0             0.64                 2
\river_model\Aberjona_Data\aberjona_gw_benzene02.dat
```

2–3. Parameter File for Methyl *tert*-Butyl Ether with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)   Depth(m)   Width(m)    Flow(m3/s)    Conc.(ug/L)
 1    0.0          0.0         0.30       5.5         0.354         0.63
 2    0.0          0.096       0.30       5.5         0.037         0.34
 3    0.096        0.096       0.53       7.3         0.0           0.00
 4    0.096        0.400       0.53       7.3         0.023         0.00
 5    0.400        0.400       0.76       7.9         0.0           0.00
 6    0.400        0.540       0.76       7.9         0.093         0.00
 7    0.540        0.540       0.34      22.8         0.0           0.00
 8    0.540        1.09        0.34      22.8        -0.173         0.00
 9    1.09         1.09        0.64       8.5         0.0           0.00
10    1.09         1.15        0.64       8.5         0.054         0.00
11    1.15         1.15        0.79       7.3         0.0           0.00
12    1.15         1.23        0.79       7.3        -0.059         0.00
13    1.23         1.23        0.37       3.6         0.0           0.00
14    1.23         1.647       0.37       3.6        -0.026         0.00
15    1.647        1.647       2.0      100.0         0.202         4.12
16    1.647        1.897       2.0      100.0         0.016         0.00
17    1.897        1.897       2.0       10.0         0.0           0.00
18    1.897        2.147       2.0       10.0         0.0           0.00
19    2.147        2.147       2.0       90.0         0.0           0.00
20    2.147        2.293       2.0       90.0         0.012         0.00
21    2.293        2.293       1.07      10.7         0.0           0.00
22    2.293        2.736       1.07      10.7         0.031         1.36
23    2.736        2.736       0.64       7.9         0.0           0.00
24    2.736        2.811       0.64       7.9         0.051         0.00
25    2.811        2.811       0.64       7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.264
 VOC molecular weight in g/mole
       88.15
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       129.39999
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
       0.184000E+02      0.766600E+04
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
MTBE~with~7-11-01~groundwater~flows
Groundwater~sources~included
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)  length   height  silldepth(m)   Tailstockdepth(m)   Type
 1          2.293        10      0.9       0.0              1.07            1
 2          2.740         5      0.5       0.0              0.64            2
\river_model\Aberjona_Data\aberjona_gw_mtbe02.dat
```

2–4. Parameter File for Chloroform with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1       0       0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)   Depth(m)    Width(m)     Flow(m³/s)    Conc.(ug/L)
 1     0.0         0.0        0.30        5.5          0.354         0.117
 2     0.0         0.096      0.30        5.5          0.037         0.00
 3     0.096       0.096      0.53        7.3          0.0           0.00
 4     0.096       0.400      0.53        7.3          0.023         0.00
 5     0.400       0.400      0.76        7.9          0.0           0.00
 6     0.400       0.540      0.76        7.9          0.093         1.16
 7     0.540       0.540      0.34        22.8         0.0           0.00
 8     0.540       1.09       0.34        22.8        -0.173         0.00
 9     1.09        1.09       0.64        8.5          0.0           0.00
10     1.09        1.15       0.64        8.5          0.054         0.00
11     1.15        1.15       0.79        7.3          0.0           0.00
12     1.15        1.23       0.79        7.3         -0.059         0.00
13     1.23        1.23       0.37        3.6          0.0           0.00
14     1.23        1.647      0.37        3.6         -0.026         0.00
15     1.647       1.647      2.0         100.0        0.202         0.00
16     1.647       1.897      2.0         100.0        0.016         0.00
17     1.897       1.897      2.0         10.0         0.0           0.00
18     1.897       2.147      2.0         10.0         0.0           0.00
19     2.147       2.147      2.0         90.0         0.0           0.00
20     2.147       2.293      2.0         90.0         0.012         0.00
21     2.293       2.293      1.07        10.7         0.0           0.00
22     2.293       2.736      1.07        10.7         0.031         0.00
23     2.736       2.736      0.64        7.9          0.0           0.00
24     2.736       2.811      0.64        7.9          0.051         0.38
25     2.811       2.811      0.64        7.9          0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.045
 VOC molecular weight in g/mole
       119.38
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       84.9325
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
9.824  4608
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
Chloroform~with~7-11-01~groundwater~flows
Groundwater~sources~included~chloroform
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1        2.293          10       0.9       0.0              1.07              1
 2        2.740           5       0.5       0.0              0.64              2
\river_model\Aberjona_Data\aberjona_gw_chloroform02.dat
```

2–5. Parameter File for 1,1-Dichloroethane with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1       0       0
Total Length of River (km)
       2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)   Depth(m)    Width(m)     Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0        0.30        5.5          0.354         0.038
 2    0.0          0.096      0.30        5.5          0.037         0.48
 3    0.096        0.096      0.53        7.3          0.0           0.00
 4    0.096        0.400      0.53        7.3          0.023         0.00
 5    0.400        0.400      0.76        7.9          0.0           0.00
 6    0.400        0.540      0.76        7.9          0.093         0.00
 7    0.540        0.540      0.34        22.8         0.0           0.00
 8    0.540        1.09       0.34        22.8         -0.173        0.00
 9    1.09         1.09       0.64        8.5          0.0           0.00
10    1.09         1.15       0.64        8.5          0.054         0.12
11    1.15         1.15       0.79        7.3          0.0           0.00
12    1.15         1.23       0.79        7.3          -0.059        0.00
13    1.23         1.23       0.37        3.6          0.0           0.00
14    1.23         1.647      0.37        3.6          -0.026        0.00
15    1.647        1.647      2.0         100.0        0.202         0.00
16    1.647        1.897      2.0         100.0        0.016         0.00
17    1.897        1.897      2.0         10.0         0.0           0.00
18    1.897        2.147      2.0         10.0         0.0           0.00
19    2.147        2.147      2.0         90.0         0.0           0.00
20    2.147        2.293      2.0         90.0         0.012         0.00
21    2.293        2.293      1.07        10.7         0.0           0.00
22    2.293        2.736      1.07        10.7         0.031         0.00
23    2.736        2.736      0.64        7.9          0.0           0.00
24    2.736        2.811      0.64        7.9          0.051         0.00
25    2.811        2.811      0.64        7.9          0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.000
 VOC molecular weight in g/mole
       98.96
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       88.849
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
        8.644               4131
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
1,1-Dichloroethane~with~7-11-01~groundwater~flows
Groundwater~sources~included~11dichloroethane
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1         2.293         10       0.9        0.0               1.07           1
 2         2.740          5       0.5        0.0               0.64           2
\river_model\Aberjona_Data\aberjona_gw_dcethane02.dat
```

2–6. Parameter File for *cis*-1,2-Dichloroethene with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1       0       0
Total Length of River (km)
        2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1     0.0         0.0         0.30        5.5         0.354         0.302
 2     0.0         0.096       0.30        5.5         0.037         0.23
 3     0.096       0.096       0.53        7.3         0.0           0.00
 4     0.096       0.400       0.53        7.3         0.023         0.00
 5     0.400       0.400       0.76        7.9         0.0           0.00
 6     0.400       0.540       0.76        7.9         0.093         0.00
 7     0.540       0.540       0.34       22.8         0.0           0.00
 8     0.540       1.09        0.34       22.8        -0.173         0.00
 9     1.09        1.09        0.64        8.5         0.0           0.00
10     1.09        1.15        0.64        8.5         0.054         0.12
11     1.15        1.15        0.79        7.3         0.0           0.00
12     1.15        1.23        0.79        7.3        -0.059         0.00
13     1.23        1.23        0.37        3.6         0.0           0.00
14     1.23        1.647       0.37        3.6        -0.026         0.00
15     1.647       1.647       2.0       100.0         0.202         0.032
16     1.647       1.897       2.0       100.0         0.016         0.00
17     1.897       1.897       2.0        10.0         0.0           0.00
18     1.897       2.147       2.0        10.0         0.0           0.00
19     2.147       2.147       2.0        90.0         0.0           0.00
20     2.147       2.293       2.0        90.0         0.012         0.00
21     2.293       2.293       1.07       10.7         0.0           0.00
22     2.293       2.736       1.07       10.7         0.031         0.33
23     2.736       2.736       0.64        7.9         0.0           0.00
24     2.736       2.811       0.64        7.9         0.051         0.00
25     2.811       2.811       0.64        7.9         0.0           0.00
 River temperatures (C)
        22.00
 Air temperature (C)
        20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.000
 VOC molecular weight in g/mole
        96.94
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
        78.087
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
8.484  4196
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
DCE~with~7-11-01~groundwater~flows
Groundwater~sources~included~dichloroethene
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)  length   height  silldepth(m)   Tailstockdepth(m)   Type
 1         2.293        10       0.9       0.0             1.07              1
 2         2.740         5       0.5       0.0             0.64              2
\river_model\Aberjona_Data\aberjona_gw_dce02.dat
```

2–7. Parameter File for Trichloroethene with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1       0       0
Total Length of River (km)
       2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)   Stop(km)   Depth(m)   Width(m)    Flow(m^3/s)   Conc.(ug/L)
 1    0.0         0.0        0.30       5.5         0.354         0.174
 2    0.0         0.096      0.30       5.5         0.037         0.21
 3    0.096       0.096      0.53       7.3         0.0           0.00
 4    0.096       0.400      0.53       7.3         0.023         0.00
 5    0.400       0.400      0.76       7.9         0.0           0.00
 6    0.400       0.540      0.76       7.9         0.093         0.39
 7    0.540       0.540      0.34       22.8        0.0           0.00
 8    0.540       1.09       0.34       22.8        -0.173        0.00
 9    1.09        1.09       0.64       8.5         0.0           0.00
10    1.09        1.15       0.64       8.5         0.054         1.09
11    1.15        1.15       0.79       7.3         0.0           0.00
12    1.15        1.23       0.79       7.3         -0.059        0.00
13    1.23        1.23       0.37       3.6         0.0           0.00
14    1.23        1.647      0.37       3.6         -0.026        0.00
15    1.647       1.647      2.0        100.0       0.202         0.035
16    1.647       1.897      2.0        100.0       0.016         0.00
17    1.897       1.897      2.0        10.0        0.0           0.00
18    1.897       2.147      2.0        10.0        0.0           0.00
19    2.147       2.147      2.0        90.0        0.0           0.00
20    2.147       2.293      2.0        90.0        0.012         0.00
21    2.293       2.293      1.07       10.7        0.0           0.00
22    2.293       2.736      1.07       10.7        0.031         0.00
23    2.736       2.736      0.64       7.9         0.0           0.00
24    2.736       2.811      0.64       7.9         0.051         0.00
25    2.811       2.811      0.64       7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.014
 VOC molecular weight in g/mole
       131.29
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       94.27
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
7.854 3702
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
TCE~with~7-11-01~groundwater~flows
Groundwater~sources~included
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#    Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1          2.293        10       0.9      0.0            1.07                1
 2          2.740         5       0.5      0.0            0.64                2
\river_model\Aberjona_Data\aberjona_gw_tce02.dat
```

2–8. Parameter File for Perchloroethene with Source Synoptic Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0         0.30        5.5         0.354         0.039
 2    0.0          0.096       0.30        5.5         0.037         0.00
 3    0.096        0.096       0.53        7.3         0.0           0.00
 4    0.096        0.400       0.53        7.3         0.023         0.00
 5    0.400        0.400       0.76        7.9         0.0           0.00
 6    0.400        0.540       0.76        7.9         0.093         0.82
 7    0.540        0.540       0.34        22.8        0.0           0.00
 8    0.540        1.09        0.34        22.8        -0.173        0.00
 9    1.09         1.09        0.64        8.5         0.0           0.00
10    1.09         1.15        0.64        8.5         0.054         0.00
11    1.15         1.15        0.79        7.3         0.0           0.00
12    1.15         1.23        0.79        7.3         -0.059        0.00
13    1.23         1.23        0.37        3.6         0.0           0.00
14    1.23         1.647       0.37        3.6         -0.026        0.00
15    1.647        1.647       2.0         100.0       0.202         0.00
16    1.647        1.897       2.0         100.0       0.016         0.00
17    1.897        1.897       2.0         10.0        0.0           0.00
18    1.897        2.147       2.0         10.0        0.0           0.00
19    2.147        2.147       2.0         90.0        0.0           0.00
20    2.147        2.293       2.0         90.0        0.012         0.00
21    2.293        2.293       1.07        10.7        0.0           0.00
22    2.293        2.736       1.07        10.7        0.031         0.00
23    2.736        2.736       0.64        7.9         0.0           0.00
24    2.736        2.811       0.64        7.9         0.051         0.00
25    2.811        2.811       0.64        7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.073
 VOC molecular weight in g/mole
       165.83
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
       115.28
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
12.484 4931
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
      0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
PCE~with~7-11-01~groundwater~flows
Groundwater~sources~included
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#    Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1          2.293         10      0.9        0.0              1.07             1
 2          2.740          5      0.5        0.0              0.64             2
\river_model\Aberjona_Data\aberjona_gw_pce02.dat
```

2–9. Parameter File for Acetone with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0         0.30        5.5         0.354         0.557
 2    0.0          0.096       0.30        5.5         0.037         0.00
 3    0.096        0.096       0.53        7.3         0.0           0.00
 4    0.096        0.400       0.53        7.3         0.023         0.00
 5    0.400        0.400       0.76        7.9         0.0           0.00
 6    0.400        0.540       0.76        7.9         0.093         0.00
 7    0.540        0.540       0.34        22.8        0.0           0.00
 8    0.540        1.09        0.34        22.8        -0.173        0.00
 9    1.09         1.09        0.64        8.5         0.0           0.00
10    1.09         1.15        0.64        8.5         0.054         0.00
11    1.15         1.15        0.79        7.3         0.0           0.00
12    1.15         1.23        0.79        7.3         -0.059        0.00
13    1.23         1.23        0.37        3.6         0.0           0.00
14    1.23         1.647       0.37        3.6         -0.026        0.00
15    1.647        1.647       2.0         100.0       0.202         0.00
16    1.647        1.897       2.0         100.0       0.016         0.00
17    1.897        1.897       2.0         10.0        0.0           0.00
18    1.897        2.147       2.0         10.0        0.0           0.00
19    2.147        2.147       2.0         90.0        0.0           0.00
20    2.147        2.293       2.0         90.0        0.012         0.00
21    2.293        2.293       1.07        10.7        0.0           0.00
22    2.293        2.736       1.07        10.7        0.031         0.00
23    2.736        2.736       0.64        7.9         0.0           0.00
24    2.736        2.811       0.64        7.9         0.051         0.00
25    2.811        2.811       0.64        7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.69
 VOC molecular weight in g/mole
       58.08
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
       73.42
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
7.034  5043
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
Acetone~with~7-11-01~groundwater~flows
Groundwater~sources~included~acetone
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)  length   height   silldepth(m)   Tailstockdepth(m)   Type
  1         2.293       10       0.9        0.0              1.07            1
  2         2.740        5       0.5        0.0              0.64            2
\river_model\Aberjona_Data\aberjona_gw_acetone03.dat
```

2–10. Parameter File for Benzene with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
       1       0      0
Total Length of River (km)
       2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)   Stop(km)   Depth(m)   Width(m)   Flow(m³/s)   Conc.(ug/L)
 1    0.0         0.0        0.30       5.5        0.354        0.009
 2    0.0         0.096      0.30       5.5        0.037        0.012
 3    0.096       0.096      0.53       7.3        0.0          0.00
 4    0.096       0.400      0.53       7.3        0.023        0.0084
 5    0.400       0.400      0.76       7.9        0.0          0.00
 6    0.400       0.540      0.76       7.9        0.093        0.013
 7    0.540       0.540      0.34       22.8       0.0          0.00
 8    0.540       1.09       0.34       22.8       -0.173       0.00
 9    1.09        1.09       0.64       8.5        0.0          0.00
10    1.09        1.15       0.64       8.5        0.054        0.0046
11    1.15        1.15       0.79       7.3        0.0          0.00
12    1.15        1.23       0.79       7.3        -0.059       0.00
13    1.23        1.23       0.37       3.6        0.0          0.00
14    1.23        1.647      0.37       3.6        -0.026       0.00
15    1.647       1.647      2.00       100.0      0.202        0.054
16    1.647       1.897      2.00       100.0      0.016        0.00
17    1.897       1.897      2.0        10.0       0.0          0.00
18    1.897       2.147      2.0        10.0       0.0          0.00
19    2.147       2.147      2.0        90.0       0.0          0.00
20    2.147       2.293      2.0        90.0       0.012        0.00
21    2.293       2.293      1.07       10.7       0.0          0.00
22    2.293       2.736      1.07       10.7       0.031        0.030
23    2.736       2.736      0.64       7.9        0.0          0.00
24    2.736       2.811      0.64       7.9        0.051        0.038
25    2.811       2.811      0.64       7.9        0.0          0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.20
 VOC molecular weight in g/mole
       78.12
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       94.27
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
       7.924 3918
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;August-20-2003
Benzene~with~7-11-01~groundwater~flows
Benzene~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)  length   height   silldepth(m)   Tailstockdepth(m)   Type
  1         2.293        10       0.9       0.0              1.07             1
  2         2.740         5       0.5       0.0              0.64             2
\river_model\Aberjona_Data\aberjona_gw_benzene03.dat
```

2–11. Parameter File for Methyl *tert*-Butyl Ether with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1        0       0
Total Length of River (km)
        2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)     Stop(km)    Depth(m)     Width(m)     Flow(m³/s)     Conc.(ug/L)
 1    0.0           0.0         0.30         5.5          0.354          0.63
 2    0.0           0.096       0.30         5.5          0.037          0.92
 3    0.096         0.096       0.53         7.3          0.0            0.00
 4    0.096         0.400       0.53         7.3          0.023          0.078
 5    0.400         0.400       0.76         7.9          0.0            0.00
 6    0.400         0.540       0.76         7.9          0.093          0.47
 7    0.540         0.540       0.34         22.8         0.0            0.00
 8    0.540         1.09        0.34         22.8         -0.173         0.00
 9    1.09          1.09        0.64         8.5          0.0            0.00
10    1.09          1.15        0.64         8.5          0.054          0.71
11    1.15          1.15        0.79         7.3          0.0            0.00
12    1.15          1.23        0.79         7.3          -0.059         0.00
13    1.23          1.23        0.37         3.6          0.0            0.00
14    1.23          1.647       0.37         3.6          -0.026         0.00
15    1.647         1.647       2.0          100.0        0.202          3.23
16    1.647         1.897       2.0          100.0        0.016          0.00
17    1.897         1.897       2.0          10.0         0.0            0.00
18    1.897         2.147       2.0          10.0         0.0            0.00
19    2.147         2.147       2.0          90.0         0.0            0.00
20    2.147         2.293       2.0          90.0         0.012          13.4
21    2.293         2.293       1.07         10.7         0.0            0.00
22    2.293         2.736       1.07         10.7         0.031          16.7
23    2.736         2.736       0.64         7.9          0.0            0.00
24    2.736         2.811       0.64         7.9          0.051          0.73
25    2.811         2.811       0.64         7.9          0.0            0.00
 River temperatures (C)
        22.00
 Air temperature (C)
        20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.264
 VOC molecular weight in g/mole
        88.15
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
        129.39999
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
        0.184000E+02      0.766600E+04
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
      0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
MTBE~with~7-11-01~groundwater~flows
MTBE~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1        2.293          10       0.9       0.0              1.07              1
 2        2.740           5       0.5       0.0              0.64              2
\river_model\Aberjona_Data\aberjona_gw_mtbe03.dat
```

2–12. Parameter File for Chloroform with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
        2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)   Stop(km)  Depth(m)   Width(m)    Flow(m³/s)   Conc.(ug/L)
 1    0.0         0.0        0.30       5.5         0.354        0.117
 2    0.0         0.096      0.30       5.5         0.037        0.19
 3    0.096       0.096      0.53       7.3         0.0          0.00
 4    0.096       0.400      0.53       7.3         0.023        0.20
 5    0.400       0.400      0.76       7.9         0.0          0.00
 6    0.400       0.540      0.76       7.9         0.093        0.19
 7    0.540       0.540      0.34       22.8        0.0          0.00
 8    0.540       1.09       0.34       22.8        -0.173       0.00
 9    1.09        1.09       0.64       8.5         0.0          0.00
10    1.09        1.15       0.64       8.5         0.054        0.26
11    1.15        1.15       0.79       7.3         0.0          0.00
12    1.15        1.23       0.79       7.3         -0.059       0.00
13    1.23        1.23       0.37       3.6         0.0          0.00
14    1.23        1.647      0.37       3.6         -0.026       0.00
15    1.647       1.647      2.00       100.0       0.202        0.16
16    1.647       1.897      2.00       100.0       0.016        0.00
17    1.897       1.897      2.0        10.0        0.0          0.00
18    1.897       2.147      2.0        10.0        0.0          0.00
19    2.147       2.147      2.0        90.0        0.0          0.00
20    2.147       2.293      2.0        90.0        0.012        2.82
21    2.293       2.293      1.07       10.7        0.0          0.00
22    2.293       2.736      1.07       10.7        0.031        0.56
23    2.736       2.736      0.64       7.9         0.0          0.00
24    2.736       2.811      0.64       7.9         0.051        0.00
25    2.811       2.811      0.64       7.9         0.0          0.00
 River temperatures (C)
        22.00
 Air temperature (C)
        20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.045
 VOC molecular weight in g/mole
        119.38
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
        84.9325
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
9.824  4608
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
Chloroform~with~7-11-01~groundwater~flows
Chloroform~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height  silldepth(m)   Tailstockdepth(m)   Type
 1         2.293         10       0.9       0.0             1.07             1
 2         2.740          5       0.5       0.0             0.64             2
\river_model\Aberjona_Data\aberjona_gw_chloroform03.dat
```

2–13. Parameter File for 1,1-Dichloroethane with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
        13
 Number of distributed source regions
        11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)   Depth(m)    Width(m)     Flow(m³/s)    Conc.(ug/L)
 1     0.0         0.0        0.30        5.5          0.354         0.038
 2     0.0         0.096      0.30        5.5          0.037         0.0033
 3     0.096       0.096      0.53        7.3          0.0           0.00
 4     0.096       0.400      0.53        7.3          0.023         0.26
 5     0.400       0.400      0.76        7.9          0.0           0.00
 6     0.400       0.540      0.76        7.9          0.093         0.047
 7     0.540       0.540      0.34        22.8         0.0           0.00
 8     0.540       1.09       0.34        22.8        -0.173         0.00
 9     1.09        1.09       0.64        8.5          0.0           0.00
10     1.09        1.15       0.64        8.5          0.054         0.55
11     1.15        1.15       0.79        7.3          0.0           0.00
12     1.15        1.23       0.79        7.3         -0.059         0.00
13     1.23        1.23       0.37        3.6          0.0           0.00
14     1.23        1.647      0.37        3.6         -0.026         0.00
15     1.647       1.647      2.00        100.0        0.202         0.13
16     1.647       1.897      2.00        100.0        0.016         0.00
17     1.897       1.897      2.0         10.0         0.0           0.00
18     1.897       2.147      2.0         10.0         0.0           0.00
19     2.147       2.147      2.0         90.0         0.0           0.00
20     2.147       2.293      2.0         90.0         0.012         1.15
21     2.293       2.293      1.07        10.7         0.0           0.00
22     2.293       2.736      1.07        10.7         0.031         0.36
23     2.736       2.736      0.64        7.9          0.0           0.00
24     2.736       2.811      0.64        7.9          0.051         0.00
25     2.811       2.811      0.64        7.9          0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.000
 VOC molecular weight in g/mole
       98.96
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       88.849
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
         8.644                 4131
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
1,1-Dichloroethane~with~7-11-01~groundwater~flows
1,1-Dichloroethane~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#    Location(km)   length   height   silldepth(m)    Tailstockdepth(m)   Type
 1          2.293         10       0.9        0.0               1.07            1
 2          2.740          5       0.5        0.0               0.64            2
\river_model\Aberjona_Data\aberjona_gw_dcethane03.dat
```

2–14. Parameter File for *cis*-1,2-Dichloroethene with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1       0       0
Total Length of River (km)
       2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0          0.0         0.30        5.5         0.354         0.302
 2    0.0          0.096       0.30        5.5         0.037         0.00
 3    0.096        0.096       0.53        7.3         0.0           0.00
 4    0.096        0.400       0.53        7.3         0.023         0.00
 5    0.400        0.400       0.76        7.9         0.0           0.00
 6    0.400        0.540       0.76        7.9         0.093         0.54
 7    0.540        0.540       0.34        22.8        0.0           0.00
 8    0.540        1.09        0.34        22.8        -0.173        0.00
 9    1.09         1.09        0.64        8.5         0.0           0.00
10    1.09         1.15        0.64        8.5         0.054         0.68
11    1.15         1.15        0.79        7.3         0.0           0.00
12    1.15         1.23        0.79        7.3         -0.059        0.00
13    1.23         1.23        0.37        3.6         0.0           0.00
14    1.23         1.647       0.37        3.6         -0.026        0.00
15    1.647        1.647       2.00        100.0       0.202         0.33
16    1.647        1.897       2.00        100.0       0.016         0.00
17    1.897        1.897       2.0         10.0        0.0           0.00
18    1.897        2.147       2.0         10.0        0.0           0.00
19    2.147        2.147       2.0         90.0        0.0           0.00
20    2.147        2.293       2.0         90.0        0.012         3.59
21    2.293        2.293       1.07        10.7        0.0           0.00
22    2.293        2.736       1.07        10.7        0.031         1.04
23    2.736        2.736       0.64        7.9         0.0           0.00
24    2.736        2.811       0.64        7.9         0.051         0.00
25    2.811        2.811       0.64        7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.000
 VOC molecular weight in g/mole
       96.94
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       78.087
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
8.484  4196
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
DCE~with~7-11-01~groundwater~flows
DCE~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1         2.293        10       0.9      0.0              1.07              1
 2         2.740         5       0.5      0.0              0.64              2
\river_model\Aberjona_Data\aberjona_gw_dce03.dat
```

2–15. Parameter File for Trichloroethene with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
        2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #   Start(km)   Stop(km)   Depth(m)   Width(m)   Flow(m³/s)   Conc.(ug/L)
 1    0.0        0.0        0.30       5.5        0.354        0.174
 2    0.0        0.096      0.30       5.5        0.037        0.25
 3    0.096      0.096      0.53       7.3        0.0          0.00
 4    0.096      0.400      0.53       7.3        0.023        0.14
 5    0.400      0.400      0.76       7.9        0.0          0.00
 6    0.400      0.540      0.76       7.9        0.093        0.26
 7    0.540      0.540      0.34       22.8       0.0          0.00
 8    0.540      1.09       0.34       22.8      -0.173        0.00
 9    1.09       1.09       0.64       8.5        0.0          0.00
10    1.09       1.15       0.64       8.5        0.054        1.65
11    1.15       1.15       0.79       7.3        0.0          0.00
12    1.15       1.23       0.79       7.3       -0.059        0.00
13    1.23       1.23       0.37       3.6        0.0          0.00
14    1.23       1.647      0.37       3.6       -0.026        0.00
15    1.647      1.647      2.0        100.0      0.202        0.34
16    1.647      1.897      2.0        100.0      0.016        0.00
17    1.897      1.897      2.0        10.0       0.0          0.00
18    1.897      2.147      2.0        10.0       0.0          0.00
19    2.147      2.147      2.0        90.0       0.0          0.00
20    2.147      2.293      2.0        90.0       0.012        6.45
21    2.293      2.293      1.07       10.7       0.0          0.00
22    2.293      2.736      1.07       10.7       0.031        0.65
23    2.736      2.736      0.64       7.9        0.0          0.00
24    2.736      2.811      0.64       7.9        0.051        0.19
25    2.811      2.811      0.64       7.9        0.0          0.00
 River temperatures (C)
        22.00
 Air temperature (C)
        20.0
 Mean wind speed (m/s)
        4.0
 Relative Humidity
        0.80
 Barometric pressure (atm)
        0.983
 Atmospheric VOC concentration (ppbv)
        0.014
 VOC molecular weight in g/mole
        131.29
 Index for molar volume data entry (1 for m.v., 2 for density)
        1
 Molar volume in ml/mol at boiling point for Wilke Chang
        94.27
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
        1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
7.854 3702
 First order VOC biochemical degradation rate (1/s)
        0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
TCE~with~7-11-01~groundwater~flows
TCE~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1         2.293         10       0.9       0.0             1.07              1
 2         2.740          5       0.5       0.0             0.64              2
\river_model\Aberjona_Data\aberjona_gw_tce03.dat
```

2–16. Parameter File for Perchloroethene with Modified Best-Fit Inputs

```
Flux Method (0 = Net, 1 = Component): Weir Flow (0=Off, 1=On): Units (0=cubic meters per second,
1=cubic feet per minute)
        1      0      0
Total Length of River (km)
       2.811
 Number of reaches
       13
 Number of distributed source regions
       11
 River profile/source data (# of points = # of reaches + # of distributed sources + 1)
 #    Start(km)    Stop(km)    Depth(m)    Width(m)    Flow(m³/s)    Conc.(ug/L)
 1    0.0         0.0         0.30        5.5         0.354         0.039
 2    0.0         0.096       0.30        5.5         0.037         0.14
 3    0.096       0.096       0.53        7.3         0.0           0.00
 4    0.096       0.400       0.53        7.3         0.023         1.08
 5    0.400       0.400       0.76        7.9         0.0           0.00
 6    0.400       0.540       0.76        7.9         0.093         0.21
 7    0.540       0.540       0.34        22.8        0.0           0.00
 8    0.540       1.09        0.34        22.8        -0.173        0.00
 9    1.09        1.09        0.64        8.5         0.0           0.00
10    1.09        1.15        0.64        8.5         0.054         0.64
11    1.15        1.15        0.79        7.3         0.0           0.00
12    1.15        1.23        0.79        7.3         -0.059        0.00
13    1.23        1.23        0.37        3.6         0.0           0.00
14    1.23        1.647       0.37        3.6         -0.026        0.00
15    1.647       1.647       2.00        100.0       0.202         0.091
16    1.647       1.897       2.00        100.0       0.016         0.00
17    1.897       1.897       2.0         10.0        0.0           0.00
18    1.897       2.147       2.0         10.0        0.0           0.00
19    2.147       2.147       2.0         90.0        0.0           0.00
20    2.147       2.293       2.0         90.0        0.012         8.78
21    2.293       2.293       1.07        10.7        0.0           0.00
22    2.293       2.736       1.07        10.7        0.031         1.53
23    2.736       2.736       0.64        7.9         0.0           0.00
24    2.736       2.811       0.64        7.9         0.051         0.11
25    2.811       2.811       0.64        7.9         0.0           0.00
 River temperatures (C)
       22.00
 Air temperature (C)
       20.0
 Mean wind speed (m/s)
       4.0
 Relative Humidity
       0.80
 Barometric pressure (atm)
       0.983
 Atmospheric VOC concentration (ppbv)
       0.073
 VOC molecular weight in g/mole
       165.83
 Index for molar volume data entry (1 for m.v., 2 for density)
       1
 Molar volume in ml/mol at boiling point for Wilke Chang
       115.28
 Solubility parameterization (1 for exp(A-B/T), 2 for Wanninkhof, 3 for direct entry)
       1
 Coefficients to give solubility in mol/m^3-atm (2 for exp(A-B/T), 5 for Wanninkhof)
12.484 4931
 First order VOC biochemical degradation rate (1/s)
       0.0
 Tolerance for Runge-Kutta DEQ integrator
     0.1000E-09
 Title for run and two lines of comments, comments not used
StreamVOC~Version~2.0;~Aberjona~River~Data;July-11-2001
PCE~with~7-11-01~groundwater~flows
PCE~sources~optimized~with~no~flow~under~weir
  end of original input file, begin waterfall/weir parameterization information
  Number of weirs/waterfalls
  2
Type:  1 = Ogee weir;2 = sharp-crested weir;3 = gated sill
Weir#   Location(km)   length   height   silldepth(m)   Tailstockdepth(m)   Type
 1        2.293          10       0.9       0.0              1.07              1
 2        2.740           5       0.5       0.0              0.64              2
\river_model\Aberjona_Data\aberjona_gw_pce03.dat
```

Appendix 3. StreamVOC Model Output Files

Definitions of Column Headings for Tables 3–1 to 3–8

x longitudinal distance along a stream
c_i concentration of contaminant
Q discharge
V velocity
k_{OL} local transfer velocity
$m_{i,in}$ total input rate from all local sources
c_s saturation concentration
ID   source identifier (1 = initial source)
km   kilometers
µg/L   micrograms per liter
m³/s   cubic meters per second
m/s   meters per second
µg   micrograms

Table 3–1. Acetone output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
							Source apportionment						
0.0000	5.57E-01	0.3542	0.215	9.19E-06	2.84E-09	9.14E-01	2	0.999	0.001	0.000	0.000	0.000	0.000
0.0132	5.75E-01	0.3593	0.218	9.21E-06	2.84E-09	9.14E-01	2	0.954	0.045	0.000	0.000	0.000	0.001
0.0265	5.93E-01	0.3643	0.221	9.23E-06	2.84E-09	9.14E-01	2	0.913	0.085	0.000	0.000	0.000	0.002
0.0397	6.10E-01	0.3694	0.224	9.25E-06	2.84E-09	9.14E-01	2	0.875	0.122	0.000	0.000	0.000	0.003
0.0529	6.26E-01	0.3745	0.227	9.27E-06	2.84E-09	9.14E-01	2	0.841	0.156	0.000	0.000	0.000	0.004
0.0662	6.43E-01	0.3796	0.230	9.29E-06	2.84E-09	9.14E-01	2	0.809	0.187	0.000	0.000	0.000	0.004
0.0794	6.58E-01	0.3847	0.233	9.31E-06	2.84E-09	9.14E-01	2	0.779	0.216	0.000	0.000	0.000	0.005
0.0926	6.73E-01	0.3897	0.236	9.33E-06	2.84E-09	9.14E-01	2	0.752	0.243	0.000	0.000	0.000	0.005
0.1062	6.76E-01	0.3914	0.101	7.02E-06	0.00E+00	9.14E-01	0	0.745	0.249	0.000	0.000	0.000	0.006
0.1197	6.75E-01	0.3924	0.101	7.03E-06	0.00E+00	9.14E-01	0	0.745	0.249	0.000	0.000	0.000	0.007
0.1332	6.74E-01	0.3934	0.102	7.03E-06	0.00E+00	9.14E-01	0	0.744	0.249	0.000	0.000	0.000	0.007
0.1467	6.72E-01	0.3944	0.102	7.04E-06	0.00E+00	9.14E-01	0	0.744	0.249	0.000	0.000	0.000	0.008
0.1602	6.71E-01	0.3955	0.102	7.04E-06	0.00E+00	9.14E-01	0	0.743	0.248	0.000	0.000	0.000	0.008
0.1737	6.70E-01	0.3965	0.103	7.04E-06	0.00E+00	9.14E-01	0	0.743	0.248	0.000	0.000	0.000	0.009
0.1872	6.68E-01	0.3975	0.103	7.05E-06	0.00E+00	9.14E-01	0	0.742	0.248	0.000	0.000	0.000	0.010
0.2007	6.67E-01	0.3986	0.103	7.05E-06	0.00E+00	9.14E-01	0	0.742	0.248	0.000	0.000	0.000	0.010
0.2142	6.66E-01	0.3995	0.103	7.06E-06	0.00E+00	9.14E-01	0	0.741	0.248	0.000	0.000	0.000	0.011
0.2276	6.65E-01	0.4006	0.104	7.06E-06	0.00E+00	9.14E-01	0	0.741	0.248	0.000	0.000	0.000	0.012
0.2411	6.63E-01	0.4016	0.104	7.07E-06	0.00E+00	9.14E-01	0	0.740	0.247	0.000	0.000	0.000	0.012
0.2546	6.62E-01	0.4026	0.104	7.07E-06	0.00E+00	9.14E-01	0	0.740	0.247	0.000	0.000	0.000	0.013
0.2681	6.61E-01	0.4037	0.104	7.08E-06	0.00E+00	9.14E-01	0	0.739	0.247	0.000	0.000	0.000	0.014
0.2816	6.60E-01	0.4047	0.105	7.08E-06	0.00E+00	9.14E-01	0	0.739	0.247	0.000	0.000	0.000	0.014
0.2951	6.58E-01	0.4057	0.105	7.08E-06	0.00E+00	9.14E-01	0	0.739	0.247	0.000	0.000	0.000	0.015
0.3086	6.57E-01	0.4067	0.105	7.09E-06	0.00E+00	9.14E-01	0	0.738	0.247	0.000	0.000	0.000	0.016
0.3221	6.56E-01	0.4078	0.105	7.09E-06	0.00E+00	9.14E-01	0	0.738	0.246	0.000	0.000	0.000	0.016
0.3356	6.55E-01	0.4087	0.106	7.10E-06	0.00E+00	9.14E-01	0	0.737	0.246	0.000	0.000	0.000	0.017
0.3490	6.54E-01	0.4098	0.106	7.10E-06	0.00E+00	9.14E-01	0	0.737	0.246	0.000	0.000	0.000	0.018
0.3625	6.52E-01	0.4108	0.106	7.11E-06	0.00E+00	9.14E-01	0	0.736	0.246	0.000	0.000	0.000	0.018
0.3760	6.51E-01	0.4118	0.106	7.11E-06	0.00E+00	9.14E-01	0	0.736	0.246	0.000	0.000	0.000	0.019
0.3895	6.50E-01	0.4129	0.107	7.11E-06	0.00E+00	9.14E-01	0	0.735	0.246	0.000	0.000	0.000	0.020
0.4025	6.49E-01	0.4136	0.084	6.37E-06	0.00E+00	9.14E-01	0	0.735	0.245	0.000	0.000	0.000	0.020
0.4158	6.38E-01	0.4213	0.070	5.79E-06	0.00E+00	9.14E-01	0	0.734	0.245	0.000	0.000	0.000	0.021
0.4290	6.25E-01	0.4303	0.072	5.82E-06	0.00E+00	9.14E-01	0	0.734	0.245	0.000	0.000	0.000	0.021
0.4422	6.12E-01	0.4393	0.073	5.86E-06	0.00E+00	9.14E-01	0	0.733	0.245	0.000	0.000	0.000	0.022
0.4554	6.01E-01	0.4484	0.075	5.89E-06	0.00E+00	9.14E-01	0	0.733	0.245	0.000	0.000	0.000	0.023
0.4686	5.89E-01	0.4575	0.076	5.93E-06	0.00E+00	9.14E-01	0	0.732	0.245	0.000	0.000	0.000	0.023
0.4818	5.78E-01	0.4665	0.078	5.96E-06	0.00E+00	9.14E-01	0	0.732	0.244	0.000	0.000	0.000	0.024
0.4950	5.68E-01	0.4757	0.079	5.99E-06	0.00E+00	9.14E-01	0	0.731	0.244	0.000	0.000	0.000	0.025
0.5082	5.57E-01	0.4847	0.081	6.02E-06	0.00E+00	9.14E-01	0	0.730	0.244	0.000	0.000	0.000	0.026
0.5214	5.48E-01	0.4937	0.082	6.05E-06	0.00E+00	9.14E-01	0	0.730	0.244	0.000	0.000	0.000	0.027
0.5346	5.38E-01	0.5026	0.084	6.08E-06	0.00E+00	9.14E-01	0	0.729	0.244	0.000	0.000	0.000	0.027
0.5477	5.35E-01	0.5050	0.065	7.03E-06	0.00E+00	9.14E-01	0	0.728	0.243	0.000	0.000	0.000	0.029
0.5614	5.37E-01	0.5007	0.065	7.02E-06	0.00E+00	9.14E-01	0	0.726	0.242	0.000	0.000	0.000	0.032
0.5750	5.39E-01	0.4960	0.064	7.00E-06	0.00E+00	9.14E-01	0	0.723	0.242	0.000	0.000	0.000	0.035
0.5887	5.40E-01	0.4918	0.064	6.99E-06	0.00E+00	9.14E-01	0	0.721	0.241	0.000	0.000	0.000	0.038
0.6024	5.42E-01	0.4875	0.063	6.97E-06	0.00E+00	9.14E-01	0	0.719	0.240	0.000	0.000	0.000	0.041
0.6160	5.44E-01	0.4833	0.062	6.96E-06	0.00E+00	9.14E-01	0	0.717	0.240	0.000	0.000	0.000	0.044

Table 3–1. Acetone output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
							Source apportionment						
0.6297	5.45E-01	0.4790	0.062	6.94E-06	0.00E+00	9.14E-01	0	0.715	0.239	0.000	0.000	0.000	0.047
0.6433	5.47E-01	0.4743	0.061	6.92E-06	0.00E+00	9.14E-01	0	0.713	0.238	0.000	0.000	0.000	0.050
0.6570	5.49E-01	0.4702	0.061	6.91E-06	0.00E+00	9.14E-01	0	0.710	0.237	0.000	0.000	0.000	0.052
0.6707	5.50E-01	0.4659	0.060	6.89E-06	0.00E+00	9.14E-01	0	0.708	0.237	0.000	0.000	0.000	0.055
0.6843	5.52E-01	0.4615	0.060	6.88E-06	0.00E+00	9.14E-01	0	0.706	0.236	0.000	0.000	0.000	0.058
0.6980	5.54E-01	0.4572	0.059	6.86E-06	0.00E+00	9.14E-01	0	0.704	0.235	0.000	0.000	0.000	0.061
0.7116	5.55E-01	0.4529	0.058	6.84E-06	0.00E+00	9.14E-01	0	0.702	0.234	0.000	0.000	0.000	0.064
0.7253	5.57E-01	0.4485	0.058	6.83E-06	0.00E+00	9.14E-01	0	0.700	0.234	0.000	0.000	0.000	0.067
0.7390	5.59E-01	0.4442	0.057	6.81E-06	0.00E+00	9.14E-01	0	0.698	0.233	0.000	0.000	0.000	0.070
0.7526	5.60E-01	0.4399	0.057	6.79E-06	0.00E+00	9.14E-01	0	0.695	0.232	0.000	0.000	0.000	0.072
0.7663	5.62E-01	0.4356	0.056	6.78E-06	0.00E+00	9.14E-01	0	0.693	0.232	0.000	0.000	0.000	0.075
0.7799	5.64E-01	0.4312	0.056	6.76E-06	0.00E+00	9.14E-01	0	0.691	0.231	0.000	0.000	0.000	0.078
0.7936	5.66E-01	0.4269	0.055	6.74E-06	0.00E+00	9.14E-01	0	0.689	0.230	0.000	0.000	0.000	0.081
0.8073	5.67E-01	0.4225	0.055	6.73E-06	0.00E+00	9.14E-01	0	0.687	0.230	0.000	0.000	0.000	0.084
0.8209	5.69E-01	0.4182	0.054	6.71E-06	0.00E+00	9.14E-01	0	0.685	0.229	0.000	0.000	0.000	0.086
0.8346	5.71E-01	0.4139	0.053	6.69E-06	0.00E+00	9.14E-01	0	0.683	0.228	0.000	0.000	0.000	0.089
0.8482	5.72E-01	0.4096	0.053	6.67E-06	0.00E+00	9.14E-01	0	0.681	0.227	0.000	0.000	0.000	0.092
0.8619	5.74E-01	0.4052	0.052	6.65E-06	0.00E+00	9.14E-01	0	0.679	0.227	0.000	0.000	0.000	0.095
0.8756	5.76E-01	0.4009	0.052	6.64E-06	0.00E+00	9.14E-01	0	0.677	0.226	0.000	0.000	0.000	0.097
0.8892	5.78E-01	0.3966	0.051	6.62E-06	0.00E+00	9.14E-01	0	0.675	0.225	0.000	0.000	0.000	0.100
0.9029	5.79E-01	0.3922	0.051	6.60E-06	0.00E+00	9.14E-01	0	0.673	0.225	0.000	0.000	0.000	0.103
0.9165	5.81E-01	0.3879	0.050	6.58E-06	0.00E+00	9.14E-01	0	0.671	0.224	0.000	0.000	0.000	0.105
0.9302	5.83E-01	0.3836	0.050	7.05E-06	0.00E+00	9.14E-01	0	0.668	0.223	0.000	0.000	0.000	0.108
0.9438	5.85E-01	0.3793	0.049	7.03E-06	0.00E+00	9.14E-01	0	0.666	0.223	0.000	0.000	0.000	0.111
0.9575	5.87E-01	0.3749	0.048	7.00E-06	0.00E+00	9.14E-01	0	0.664	0.222	0.000	0.000	0.000	0.114
0.9712	5.89E-01	0.3706	0.048	6.97E-06	0.00E+00	9.14E-01	0	0.662	0.221	0.000	0.000	0.000	0.117
0.9848	5.91E-01	0.3662	0.047	6.94E-06	0.00E+00	9.14E-01	0	0.660	0.220	0.000	0.000	0.000	0.120
0.9985	5.93E-01	0.3619	0.047	6.91E-06	0.00E+00	9.14E-01	0	0.658	0.220	0.000	0.000	0.000	0.123
1.0121	5.94E-01	0.3576	0.046	6.88E-06	0.00E+00	9.14E-01	0	0.656	0.219	0.000	0.000	0.000	0.125
1.0258	5.96E-01	0.3532	0.046	6.85E-06	0.00E+00	9.14E-01	0	0.654	0.218	0.000	0.000	0.000	0.128
1.0395	5.98E-01	0.3489	0.045	6.82E-06	0.00E+00	9.14E-01	0	0.651	0.218	0.000	0.000	0.000	0.131
1.0531	6.00E-01	0.3446	0.045	6.79E-06	0.00E+00	9.14E-01	0	0.649	0.217	0.000	0.000	0.000	0.134
1.0668	6.02E-01	0.3403	0.044	6.76E-06	0.00E+00	9.14E-01	0	0.647	0.216	0.000	0.000	0.000	0.137
1.0804	6.04E-01	0.3359	0.043	6.72E-06	0.00E+00	9.14E-01	0	0.645	0.216	0.000	0.000	0.000	0.139
1.0934	6.10E-01	0.3333	0.047	5.72E-06	8.32E-11	9.14E-01	3	0.639	0.214	0.007	0.000	0.000	0.141
1.1066	6.05E-01	0.3448	0.063	5.90E-06	9.15E-10	9.14E-01	3	0.623	0.208	0.031	0.000	0.000	0.138
1.1197	5.98E-01	0.3576	0.066	5.97E-06	9.15E-10	9.14E-01	3	0.608	0.203	0.054	0.000	0.000	0.136
1.1328	5.91E-01	0.3704	0.068	6.03E-06	9.15E-10	9.14E-01	3	0.593	0.198	0.075	0.000	0.000	0.134
1.1459	5.85E-01	0.3833	0.070	6.08E-06	9.15E-10	9.14E-01	3	0.579	0.194	0.096	0.000	0.000	0.131
1.1589	5.84E-01	0.3839	0.067	5.64E-06	0.00E+00	9.14E-01	0	0.575	0.192	0.102	0.000	0.000	0.131
1.1721	5.84E-01	0.3734	0.065	5.59E-06	0.00E+00	9.14E-01	0	0.574	0.192	0.102	0.000	0.000	0.132
1.1853	5.85E-01	0.3630	0.063	5.54E-06	0.00E+00	9.14E-01	0	0.574	0.192	0.102	0.000	0.000	0.133
1.1984	5.85E-01	0.3526	0.061	5.50E-06	0.00E+00	9.14E-01	0	0.573	0.192	0.102	0.000	0.000	0.133
1.2116	5.86E-01	0.3421	0.059	5.45E-06	0.00E+00	9.14E-01	0	0.573	0.191	0.102	0.000	0.000	0.134
1.2247	5.86E-01	0.3317	0.058	5.40E-06	0.00E+00	9.14E-01	0	0.572	0.191	0.102	0.000	0.000	0.135
1.2377	5.87E-01	0.3273	0.246	9.07E-06	0.00E+00	9.14E-01	0	0.572	0.191	0.102	0.000	0.000	0.136

Table 3–1.   Acetone output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source apportionment						
							ID	1	2	3	4	5	Air
1.2512	5.87E-01	0.3265	0.245	9.07E-06	0.00E+00	9.14E-01	0	0.571	0.191	0.102	0.000	0.000	0.136
1.2647	5.88E-01	0.3256	0.245	9.07E-06	0.00E+00	9.14E-01	0	0.571	0.191	0.102	0.000	0.000	0.137
1.2782	5.88E-01	0.3247	0.244	9.06E-06	0.00E+00	9.14E-01	0	0.571	0.191	0.101	0.000	0.000	0.138
1.2916	5.89E-01	0.3239	0.243	9.06E-06	0.00E+00	9.14E-01	0	0.570	0.191	0.101	0.000	0.000	0.138
1.3051	5.89E-01	0.3230	0.243	9.05E-06	0.00E+00	9.14E-01	0	0.570	0.190	0.101	0.000	0.000	0.139
1.3186	5.89E-01	0.3221	0.242	9.05E-06	0.00E+00	9.14E-01	0	0.569	0.190	0.101	0.000	0.000	0.139
1.3320	5.90E-01	0.3213	0.241	9.05E-06	0.00E+00	9.14E-01	0	0.569	0.190	0.101	0.000	0.000	0.140
1.3455	5.90E-01	0.3204	0.241	9.04E-06	0.00E+00	9.14E-01	0	0.568	0.190	0.101	0.000	0.000	0.141
1.3590	5.91E-01	0.3196	0.240	9.04E-06	0.00E+00	9.14E-01	0	0.568	0.190	0.101	0.000	0.000	0.141
1.3724	5.91E-01	0.3187	0.239	9.03E-06	0.00E+00	9.14E-01	0	0.568	0.190	0.101	0.000	0.000	0.142
1.3859	5.92E-01	0.3179	0.239	9.03E-06	0.00E+00	9.14E-01	0	0.567	0.190	0.101	0.000	0.000	0.143
1.3994	5.92E-01	0.3170	0.238	9.03E-06	0.00E+00	9.14E-01	0	0.567	0.189	0.101	0.000	0.000	0.143
1.4128	5.93E-01	0.3162	0.237	9.02E-06	0.00E+00	9.14E-01	0	0.566	0.189	0.101	0.000	0.000	0.144
1.4263	5.93E-01	0.3153	0.237	9.02E-06	0.00E+00	9.14E-01	0	0.566	0.189	0.101	0.000	0.000	0.145
1.4398	5.93E-01	0.3144	0.236	9.01E-06	0.00E+00	9.14E-01	0	0.565	0.189	0.101	0.000	0.000	0.145
1.4533	5.94E-01	0.3136	0.235	9.01E-06	0.00E+00	9.14E-01	0	0.565	0.189	0.100	0.000	0.000	0.146
1.4667	5.94E-01	0.3127	0.235	9.00E-06	0.00E+00	9.14E-01	0	0.565	0.189	0.100	0.000	0.000	0.147
1.4802	5.95E-01	0.3118	0.234	9.00E-06	0.00E+00	9.14E-01	0	0.564	0.189	0.100	0.000	0.000	0.147
1.4937	5.95E-01	0.3110	0.234	9.00E-06	0.00E+00	9.14E-01	0	0.564	0.188	0.100	0.000	0.000	0.148
1.5071	5.96E-01	0.3101	0.233	8.99E-06	0.00E+00	9.14E-01	0	0.563	0.188	0.100	0.000	0.000	0.148
1.5206	5.96E-01	0.3093	0.232	8.99E-06	0.00E+00	9.14E-01	0	0.563	0.188	0.100	0.000	0.000	0.149
1.5341	5.97E-01	0.3084	0.232	8.98E-06	0.00E+00	9.14E-01	0	0.563	0.188	0.100	0.000	0.000	0.150
1.5475	5.97E-01	0.3075	0.231	8.98E-06	0.00E+00	9.14E-01	0	0.562	0.188	0.100	0.000	0.000	0.150
1.5610	5.97E-01	0.3067	0.230	8.97E-06	0.00E+00	9.14E-01	0	0.562	0.188	0.100	0.000	0.000	0.151
1.5745	5.98E-01	0.3058	0.230	8.97E-06	0.00E+00	9.14E-01	0	0.561	0.188	0.100	0.000	0.000	0.152
1.5879	5.98E-01	0.3049	0.229	8.97E-06	0.00E+00	9.14E-01	0	0.561	0.187	0.100	0.000	0.000	0.152
1.6014	5.99E-01	0.3041	0.228	8.96E-06	0.00E+00	9.14E-01	0	0.560	0.187	0.100	0.000	0.000	0.153
1.6149	5.99E-01	0.3032	0.228	8.96E-06	0.00E+00	9.14E-01	0	0.560	0.187	0.100	0.000	0.000	0.154
1.6284	6.00E-01	0.3024	0.227	8.95E-06	0.00E+00	9.14E-01	0	0.560	0.187	0.099	0.000	0.000	0.154
1.6418	6.00E-01	0.3015	0.226	8.95E-06	0.00E+00	9.14E-01	0	0.559	0.187	0.099	0.000	0.000	0.155
1.6551	3.63E-01	0.5036	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.554	0.185	0.098	0.000	0.000	0.163
1.6686	3.71E-01	0.5045	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.541	0.181	0.096	0.000	0.000	0.183
1.6821	3.78E-01	0.5050	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.529	0.177	0.094	0.000	0.000	0.201
1.6956	3.86E-01	0.5059	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.517	0.173	0.092	0.000	0.000	0.218
1.7091	3.94E-01	0.5069	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.507	0.169	0.090	0.000	0.000	0.234
1.7226	4.01E-01	0.5078	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.497	0.166	0.088	0.000	0.000	0.249
1.7361	4.08E-01	0.5088	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.487	0.163	0.087	0.000	0.000	0.264
1.7496	4.15E-01	0.5092	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.478	0.160	0.085	0.000	0.000	0.278
1.7631	4.22E-01	0.5102	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.469	0.157	0.083	0.000	0.000	0.291
1.7766	4.29E-01	0.5111	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.461	0.154	0.082	0.000	0.000	0.303
1.7902	4.36E-01	0.5121	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.453	0.151	0.081	0.000	0.000	0.315
1.8037	4.42E-01	0.5130	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.446	0.149	0.079	0.000	0.000	0.326
1.8172	4.49E-01	0.5139	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.439	0.147	0.078	0.000	0.000	0.337
1.8307	4.55E-01	0.5144	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.432	0.144	0.077	0.000	0.000	0.347
1.8442	4.61E-01	0.5154	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.425	0.142	0.076	0.000	0.000	0.357
1.8577	4.67E-01	0.5163	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.419	0.140	0.075	0.000	0.000	0.367
1.8712	4.73E-01	0.5172	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.413	0.138	0.073	0.000	0.000	0.376

Table 3–1. Acetone output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
							Source apportionment						
1.8847	4.79E-01	0.5182	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.407	0.136	0.072	0.000	0.000	0.384
1.8977	4.85E-01	0.5187	0.003	5.83E-06	0.00E+00	9.14E-01	0	0.402	0.134	0.072	0.000	0.000	0.392
1.9112	4.86E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.401	0.134	0.071	0.000	0.000	0.394
1.9247	4.87E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.400	0.134	0.071	0.000	0.000	0.395
1.9382	4.87E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.400	0.134	0.071	0.000	0.000	0.396
1.9517	4.88E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.399	0.133	0.071	0.000	0.000	0.396
1.9652	4.89E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.399	0.133	0.071	0.000	0.000	0.397
1.9788	4.89E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.398	0.133	0.071	0.000	0.000	0.398
1.9923	4.90E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.398	0.133	0.071	0.000	0.000	0.399
2.0058	4.91E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.397	0.133	0.071	0.000	0.000	0.400
2.0193	4.91E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.397	0.133	0.071	0.000	0.000	0.400
2.0328	4.92E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.396	0.132	0.070	0.000	0.000	0.401
2.0463	4.92E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.396	0.132	0.070	0.000	0.000	0.402
2.0598	4.93E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.395	0.132	0.070	0.000	0.000	0.403
2.0733	4.94E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.395	0.132	0.070	0.000	0.000	0.404
2.0868	4.94E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.394	0.132	0.070	0.000	0.000	0.404
2.1003	4.95E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.394	0.132	0.070	0.000	0.000	0.405
2.1138	4.96E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.393	0.131	0.070	0.000	0.000	0.406
2.1274	4.96E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.393	0.131	0.070	0.000	0.000	0.407
2.1409	4.97E-01	0.5187	0.026	5.83E-06	0.00E+00	9.14E-01	0	0.392	0.131	0.070	0.000	0.000	0.407
2.1541	5.00E-01	0.5191	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.389	0.130	0.069	0.002	0.000	0.409
2.1672	5.07E-01	0.5201	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.384	0.128	0.068	0.006	0.000	0.414
2.1803	5.13E-01	0.5210	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.378	0.126	0.067	0.010	0.000	0.418
2.1933	5.19E-01	0.5224	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.373	0.125	0.066	0.014	0.000	0.423
2.2064	5.25E-01	0.5234	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.368	0.123	0.065	0.017	0.000	0.427
2.2195	5.31E-01	0.5243	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.363	0.121	0.065	0.021	0.000	0.431
2.2326	5.37E-01	0.5257	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.358	0.120	0.064	0.024	0.000	0.434
2.2456	5.43E-01	0.5267	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.354	0.118	0.063	0.028	0.000	0.438
2.2587	5.48E-01	0.5276	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.349	0.117	0.062	0.031	0.000	0.441
2.2718	5.54E-01	0.5290	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.345	0.115	0.061	0.034	0.000	0.444
2.2849	5.59E-01	0.5300	0.003	5.83E-06	4.87E-10	9.14E-01	4	0.341	0.114	0.061	0.037	0.000	0.447
2.2979	6.02E-01	0.5305	0.039	5.83E-06	9.25E-12	9.14E-01	5	0.317	0.106	0.056	0.037	0.001	0.484
2.3112	6.02E-01	0.5314	0.046	4.11E-06	8.11E-10	9.14E-01	5	0.316	0.106	0.056	0.036	0.002	0.484
2.3243	6.02E-01	0.5324	0.047	4.11E-06	8.11E-10	9.14E-01	5	0.315	0.105	0.056	0.036	0.004	0.483
2.3375	6.03E-01	0.5333	0.047	4.12E-06	8.11E-10	9.14E-01	5	0.314	0.105	0.056	0.036	0.006	0.483
2.3507	6.03E-01	0.5342	0.047	4.12E-06	8.11E-10	9.14E-01	5	0.314	0.105	0.056	0.036	0.008	0.482
2.3639	6.03E-01	0.5352	0.047	4.12E-06	8.11E-10	9.14E-01	5	0.313	0.105	0.056	0.036	0.009	0.481
2.3770	6.04E-01	0.5361	0.047	4.13E-06	8.11E-10	9.14E-01	5	0.312	0.104	0.056	0.036	0.011	0.481
2.3902	6.04E-01	0.5371	0.047	4.13E-06	8.11E-10	9.14E-01	5	0.312	0.104	0.055	0.036	0.013	0.480
2.4034	6.04E-01	0.5380	0.047	4.14E-06	8.11E-10	9.14E-01	5	0.311	0.104	0.055	0.036	0.015	0.480
2.4166	6.05E-01	0.5390	0.047	4.14E-06	8.11E-10	9.14E-01	5	0.310	0.104	0.055	0.036	0.016	0.479
2.4297	6.05E-01	0.5399	0.047	4.14E-06	8.11E-10	9.14E-01	5	0.309	0.103	0.055	0.036	0.018	0.479
2.4429	6.05E-01	0.5408	0.047	4.15E-06	8.11E-10	9.14E-01	5	0.309	0.103	0.055	0.036	0.020	0.478
2.4561	6.06E-01	0.5418	0.047	4.15E-06	8.11E-10	9.14E-01	5	0.308	0.103	0.055	0.036	0.021	0.478
2.4692	6.06E-01	0.5427	0.047	4.15E-06	8.11E-10	9.14E-01	5	0.307	0.103	0.055	0.035	0.023	0.477
2.4824	6.06E-01	0.5437	0.047	4.16E-06	8.11E-10	9.14E-01	5	0.307	0.102	0.055	0.035	0.025	0.477
2.4956	6.07E-01	0.5446	0.048	4.16E-06	8.11E-10	9.14E-01	5	0.306	0.102	0.054	0.035	0.026	0.476

Table 3–1. Acetone output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source apportionment ID	1	2	3	4	5	Air
2.5088	6.07E-01	0.5456	0.048	4.16E-06	8.11E-10	9.14E-01	5	0.305	0.102	0.054	0.035	0.028	0.476
2.5219	6.07E-01	0.5465	0.048	4.17E-06	8.11E-10	9.14E-01	5	0.305	0.102	0.054	0.035	0.030	0.475
2.5351	6.08E-01	0.5475	0.048	4.17E-06	8.11E-10	9.14E-01	5	0.304	0.102	0.054	0.035	0.031	0.475
2.5483	6.08E-01	0.5484	0.048	4.18E-06	8.11E-10	9.14E-01	5	0.303	0.101	0.054	0.035	0.033	0.474
2.5615	6.08E-01	0.5493	0.048	4.18E-06	8.11E-10	9.14E-01	5	0.302	0.101	0.054	0.035	0.035	0.473
2.5746	6.09E-01	0.5503	0.048	4.18E-06	8.11E-10	9.14E-01	5	0.302	0.101	0.054	0.035	0.036	0.473
2.5878	6.09E-01	0.5512	0.048	4.19E-06	8.11E-10	9.14E-01	5	0.301	0.101	0.054	0.035	0.038	0.472
2.6010	6.09E-01	0.5522	0.048	4.19E-06	8.11E-10	9.14E-01	5	0.300	0.100	0.053	0.035	0.039	0.472
2.6142	6.10E-01	0.5531	0.048	4.19E-06	8.11E-10	9.14E-01	5	0.300	0.100	0.053	0.035	0.041	0.471
2.6273	6.10E-01	0.5541	0.048	4.20E-06	8.11E-10	9.14E-01	5	0.299	0.100	0.053	0.035	0.042	0.471
2.6405	6.10E-01	0.5550	0.048	4.20E-06	8.11E-10	9.14E-01	5	0.299	0.100	0.053	0.034	0.044	0.470
2.6537	6.10E-01	0.5559	0.049	4.20E-06	8.11E-10	9.14E-01	5	0.298	0.100	0.053	0.034	0.046	0.470
2.6668	6.11E-01	0.5569	0.049	4.21E-06	8.11E-10	9.14E-01	5	0.297	0.099	0.053	0.034	0.047	0.469
2.6800	6.11E-01	0.5578	0.049	4.21E-06	8.11E-10	9.14E-01	5	0.297	0.099	0.053	0.034	0.049	0.469
2.6932	6.11E-01	0.5588	0.049	4.22E-06	8.11E-10	9.14E-01	5	0.296	0.099	0.053	0.034	0.050	0.468
2.7064	6.12E-01	0.5597	0.049	4.22E-06	8.11E-10	9.14E-01	5	0.295	0.099	0.053	0.034	0.052	0.468
2.7195	6.12E-01	0.5607	0.049	4.22E-06	8.11E-10	9.14E-01	5	0.295	0.098	0.052	0.034	0.053	0.467
2.7327	6.12E-01	0.5616	0.049	4.23E-06	8.11E-10	9.14E-01	5	0.294	0.098	0.052	0.034	0.055	0.467
2.7457	6.23E-01	0.5654	0.112	6.87E-06	0.00E+00	9.14E-01	0	0.287	0.096	0.051	0.033	0.054	0.479
2.7589	6.13E-01	0.5748	0.114	6.90E-06	0.00E+00	9.14E-01	0	0.287	0.096	0.051	0.033	0.054	0.479
2.7721	6.03E-01	0.5847	0.116	6.93E-06	0.00E+00	9.14E-01	0	0.287	0.096	0.051	0.033	0.054	0.480
2.7852	5.94E-01	0.5942	0.118	6.96E-06	0.00E+00	9.14E-01	0	0.287	0.096	0.051	0.033	0.054	0.480
2.7984	5.85E-01	0.6036	0.119	6.98E-06	0.00E+00	9.14E-01	0	0.286	0.096	0.051	0.033	0.054	0.480

Table 3–2.   Benzene output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
0.0000	9.00E-03	0.3542	0.215	2.54E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0132	8.84E-03	0.3593	0.218	2.56E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0265	8.69E-03	0.3643	0.221	2.57E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0397	8.54E-03	0.3694	0.224	2.59E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0529	8.40E-03	0.3745	0.227	2.61E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0662	8.26E-03	0.3796	0.230	2.63E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0794	8.13E-03	0.3847	0.233	2.64E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.0926	8.00E-03	0.3897	0.236	2.66E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1062	7.95E-03	0.3914	0.101	1.32E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1197	7.91E-03	0.3924	0.101	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1332	7.87E-03	0.3934	0.102	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1467	7.84E-03	0.3944	0.102	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1602	7.80E-03	0.3955	0.102	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1737	7.77E-03	0.3965	0.103	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.1872	7.73E-03	0.3975	0.103	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2007	7.70E-03	0.3986	0.103	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2142	7.66E-03	0.3995	0.103	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2276	7.63E-03	0.4006	0.104	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2411	7.60E-03	0.4016	0.104	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2546	7.56E-03	0.4026	0.104	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2681	7.53E-03	0.4037	0.104	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2816	7.50E-03	0.4047	0.105	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.2951	7.46E-03	0.4057	0.105	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3086	7.43E-03	0.4067	0.105	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3221	7.40E-03	0.4078	0.105	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3356	7.37E-03	0.4087	0.106	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3490	7.33E-03	0.4098	0.106	1.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3625	7.30E-03	0.4108	0.106	1.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3760	7.27E-03	0.4118	0.106	1.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.3895	7.24E-03	0.4129	0.107	1.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4025	7.22E-03	0.4136	0.084	1.10E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4158	7.08E-03	0.4213	0.070	9.23E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4290	6.92E-03	0.4303	0.072	9.33E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4422	6.77E-03	0.4393	0.073	9.42E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4554	6.62E-03	0.4484	0.075	9.52E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4686	6.49E-03	0.4575	0.076	9.61E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4818	6.35E-03	0.4665	0.078	9.71E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.4950	6.23E-03	0.4757	0.079	9.80E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5082	6.10E-03	0.4847	0.081	9.89E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5214	5.99E-03	0.4937	0.082	9.98E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5346	5.87E-03	0.5026	0.084	1.01E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5477	5.82E-03	0.5050	0.065	1.33E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5614	5.80E-03	0.5007	0.065	1.32E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5750	5.78E-03	0.4960	0.064	1.32E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.5887	5.76E-03	0.4918	0.064	1.31E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6024	5.74E-03	0.4875	0.063	1.30E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000

Table 3–2. Benzene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
0.6160	5.72E-03	0.4833	0.062	1.30E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6297	5.70E-03	0.4790	0.062	1.29E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6433	5.68E-03	0.4743	0.061	1.29E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6570	5.65E-03	0.4702	0.061	1.28E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6707	5.63E-03	0.4659	0.060	1.27E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6843	5.61E-03	0.4615	0.060	1.27E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.6980	5.59E-03	0.4572	0.059	1.26E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7116	5.57E-03	0.4529	0.058	1.26E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7253	5.55E-03	0.4485	0.058	1.25E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7390	5.53E-03	0.4442	0.057	1.25E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7526	5.51E-03	0.4399	0.057	1.24E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7663	5.49E-03	0.4356	0.056	1.23E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7799	5.47E-03	0.4312	0.056	1.23E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.7936	5.45E-03	0.4269	0.055	1.22E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8073	5.43E-03	0.4225	0.055	1.21E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8209	5.41E-03	0.4182	0.054	1.21E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8346	5.39E-03	0.4139	0.053	1.20E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8482	5.38E-03	0.4096	0.053	1.20E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8619	5.36E-03	0.4052	0.052	1.19E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8756	5.34E-03	0.4009	0.052	1.18E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.8892	5.32E-03	0.3966	0.051	1.18E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9029	5.30E-03	0.3922	0.051	1.17E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9165	5.28E-03	0.3879	0.050	1.16E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9302	5.26E-03	0.3836	0.050	1.34E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9438	5.24E-03	0.3793	0.049	1.32E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9575	5.21E-03	0.3749	0.048	1.31E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9712	5.19E-03	0.3706	0.048	1.30E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9848	5.17E-03	0.3662	0.047	1.29E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
0.9985	5.15E-03	0.3619	0.047	1.28E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0121	5.13E-03	0.3576	0.046	1.27E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0258	5.11E-03	0.3532	0.046	1.26E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0395	5.09E-03	0.3489	0.045	1.25E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0531	5.07E-03	0.3446	0.045	1.24E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0668	5.05E-03	0.3403	0.044	1.23E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0804	5.03E-03	0.3359	0.043	1.21E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.0934	5.01E-03	0.3333	0.047	9.05E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1066	4.84E-03	0.3448	0.063	9.56E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1197	4.66E-03	0.3576	0.066	9.73E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1328	4.49E-03	0.3704	0.068	9.90E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1459	4.34E-03	0.3833	0.070	1.01E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1589	4.29E-03	0.3839	0.067	8.82E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1721	4.29E-03	0.3734	0.065	8.70E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1853	4.29E-03	0.3630	0.063	8.58E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.1984	4.29E-03	0.3526	0.061	8.46E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2116	4.28E-03	0.3421	0.059	8.33E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2247	4.28E-03	0.3317	0.058	8.21E-06	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2377	4.28E-03	0.3273	0.246	2.45E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000

Table 3–2.   Benzene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
1.2512	4.28E-03	0.3265	0.245	2.44E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2647	4.27E-03	0.3256	0.245	2.44E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2782	4.27E-03	0.3247	0.244	2.44E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.2916	4.26E-03	0.3239	0.243	2.43E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3051	4.26E-03	0.3230	0.243	2.43E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3186	4.26E-03	0.3221	0.242	2.43E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3320	4.25E-03	0.3213	0.241	2.43E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3455	4.25E-03	0.3204	0.241	2.42E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3590	4.25E-03	0.3196	0.240	2.42E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3724	4.24E-03	0.3187	0.239	2.42E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3859	4.24E-03	0.3179	0.239	2.41E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.3994	4.23E-03	0.3170	0.238	2.41E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4128	4.23E-03	0.3162	0.237	2.41E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4263	4.23E-03	0.3153	0.237	2.40E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4398	4.22E-03	0.3144	0.236	2.40E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4533	4.22E-03	0.3136	0.235	2.40E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4667	4.22E-03	0.3127	0.235	2.39E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4802	4.21E-03	0.3118	0.234	2.39E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.4937	4.21E-03	0.3110	0.234	2.39E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5071	4.21E-03	0.3101	0.233	2.38E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5206	4.20E-03	0.3093	0.232	2.38E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5341	4.20E-03	0.3084	0.232	2.38E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5475	4.19E-03	0.3075	0.231	2.37E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5610	4.19E-03	0.3067	0.230	2.37E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5745	4.19E-03	0.3058	0.230	2.37E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.5879	4.18E-03	0.3049	0.229	2.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.6014	4.18E-03	0.3041	0.228	2.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.6149	4.18E-03	0.3032	0.228	2.36E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.6284	4.17E-03	0.3024	0.227	2.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.6418	4.17E-03	0.3015	0.226	2.35E-05	0.00E+00	3.24E-03	0	1.000	0.000	0.000
1.6551	2.24E-02	0.5036	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.6686	2.19E-02	0.5045	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.6821	2.14E-02	0.5050	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.6956	2.09E-02	0.5059	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7091	2.04E-02	0.5069	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7226	2.00E-02	0.5078	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7361	1.95E-02	0.5088	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7496	1.91E-02	0.5092	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7631	1.87E-02	0.5102	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7766	1.83E-02	0.5111	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.7902	1.79E-02	0.5121	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8037	1.75E-02	0.5130	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8172	1.71E-02	0.5139	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8307	1.67E-02	0.5144	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8442	1.64E-02	0.5154	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8577	1.60E-02	0.5163	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8712	1.57E-02	0.5172	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000

Table 3–2.   Benzene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
1.8847	1.54E-02	0.5182	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.8977	1.51E-02	0.5187	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9112	1.50E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9247	1.50E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9382	1.50E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9517	1.49E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9652	1.49E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9788	1.49E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
1.9923	1.48E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0058	1.48E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0193	1.48E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0328	1.48E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0463	1.47E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0598	1.47E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0733	1.47E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.0868	1.46E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1003	1.46E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1138	1.46E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1274	1.46E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1409	1.45E-02	0.5187	0.026	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1541	1.44E-02	0.5191	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1672	1.42E-02	0.5201	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1803	1.39E-02	0.5210	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.1933	1.37E-02	0.5224	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2064	1.34E-02	0.5234	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2195	1.32E-02	0.5243	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2326	1.29E-02	0.5257	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2456	1.27E-02	0.5267	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2587	1.25E-02	0.5276	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2718	1.23E-02	0.5290	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2849	1.21E-02	0.5300	0.003	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.2979	8.98E-03	0.5305	0.039	9.34E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3112	8.96E-03	0.5314	0.046	5.42E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3243	8.93E-03	0.5324	0.047	5.43E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3375	8.91E-03	0.5333	0.047	5.44E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3507	8.89E-03	0.5342	0.047	5.44E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3639	8.86E-03	0.5352	0.047	5.45E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3770	8.84E-03	0.5361	0.047	5.46E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.3902	8.82E-03	0.5371	0.047	5.46E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4034	8.79E-03	0.5380	0.047	5.47E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4166	8.77E-03	0.5390	0.047	5.48E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4297	8.75E-03	0.5399	0.047	5.49E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4429	8.72E-03	0.5408	0.047	5.49E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4561	8.70E-03	0.5418	0.047	5.50E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4692	8.68E-03	0.5427	0.047	5.51E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4824	8.65E-03	0.5437	0.047	5.51E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.4956	8.63E-03	0.5446	0.048	5.52E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000

Table 3–2.   Benzene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
2.5088	8.61E-03	0.5456	0.048	5.53E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5219	8.59E-03	0.5465	0.048	5.53E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5351	8.56E-03	0.5475	0.048	5.54E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5483	8.54E-03	0.5484	0.048	5.55E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5615	8.52E-03	0.5493	0.048	5.55E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5746	8.50E-03	0.5503	0.048	5.56E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.5878	8.48E-03	0.5512	0.048	5.57E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6010	8.45E-03	0.5522	0.048	5.58E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6142	8.43E-03	0.5531	0.048	5.58E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6273	8.41E-03	0.5541	0.048	5.59E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6405	8.39E-03	0.5550	0.048	5.60E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6537	8.37E-03	0.5559	0.049	5.60E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6668	8.35E-03	0.5569	0.049	5.61E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6800	8.33E-03	0.5578	0.049	5.62E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.6932	8.30E-03	0.5588	0.049	5.62E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7064	8.28E-03	0.5597	0.049	5.63E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7195	8.26E-03	0.5607	0.049	5.64E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7327	8.24E-03	0.5616	0.049	5.64E-06	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7457	7.34E-03	0.5654	0.112	1.27E-05	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7589	7.20E-03	0.5748	0.114	1.28E-05	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7721	7.08E-03	0.5847	0.116	1.29E-05	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7852	6.95E-03	0.5942	0.118	1.30E-05	0.00E+00	3.24E-03	0	0.110	0.890	0.000
2.7984	6.84E-03	0.6036	0.119	1.31E-05	0.00E+00	3.24E-03	0	0.110	0.890	0.000

Table 3–3. Methyl *tert*-butyl ether output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment					
							ID	1	2	3	4	Air
0.0000	6.30E-01	0.3542	0.215	2.00E-05	3.56E-10	4.45E-02	2	1.000	0.000	0.000	0.000	0.000
0.0132	6.23E-01	0.3593	0.218	2.02E-05	3.56E-10	4.45E-02	2	0.992	0.008	0.000	0.000	0.000
0.0265	6.17E-01	0.3643	0.221	2.03E-05	3.56E-10	4.45E-02	2	0.985	0.015	0.000	0.000	0.000
0.0397	6.11E-01	0.3694	0.224	2.04E-05	3.56E-10	4.45E-02	2	0.977	0.023	0.000	0.000	0.000
0.0529	6.05E-01	0.3745	0.227	2.05E-05	3.56E-10	4.45E-02	2	0.970	0.030	0.000	0.000	0.000
0.0662	5.99E-01	0.3796	0.230	2.06E-05	3.56E-10	4.45E-02	2	0.962	0.038	0.000	0.000	0.000
0.0794	5.94E-01	0.3847	0.233	2.07E-05	3.56E-10	4.45E-02	2	0.955	0.045	0.000	0.000	0.000
0.0926	5.88E-01	0.3897	0.236	2.09E-05	3.56E-10	4.45E-02	2	0.948	0.052	0.000	0.000	0.000
0.1062	5.85E-01	0.3914	0.101	1.11E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1197	5.82E-01	0.3924	0.101	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1332	5.79E-01	0.3934	0.102	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1467	5.76E-01	0.3944	0.102	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1602	5.73E-01	0.3955	0.102	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1737	5.70E-01	0.3965	0.103	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.1872	5.67E-01	0.3975	0.103	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2007	5.64E-01	0.3986	0.103	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2142	5.62E-01	0.3995	0.103	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2276	5.59E-01	0.4006	0.104	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2411	5.56E-01	0.4016	0.104	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2546	5.53E-01	0.4026	0.104	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2681	5.50E-01	0.4037	0.104	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2816	5.47E-01	0.4047	0.105	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.2951	5.45E-01	0.4057	0.105	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3086	5.42E-01	0.4067	0.105	1.13E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3221	5.39E-01	0.4078	0.105	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3356	5.37E-01	0.4087	0.106	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3490	5.34E-01	0.4098	0.106	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3625	5.31E-01	0.4108	0.106	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3760	5.29E-01	0.4118	0.106	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.3895	5.26E-01	0.4129	0.107	1.14E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4025	5.24E-01	0.4136	0.084	9.34E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4158	5.13E-01	0.4213	0.070	7.95E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4290	5.02E-01	0.4303	0.072	8.03E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4422	4.90E-01	0.4393	0.073	8.11E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4554	4.80E-01	0.4484	0.075	8.19E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4686	4.69E-01	0.4575	0.076	8.26E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4818	4.60E-01	0.4665	0.078	8.34E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.4950	4.50E-01	0.4757	0.079	8.42E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5082	4.41E-01	0.4847	0.081	8.49E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5214	4.32E-01	0.4937	0.082	8.56E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5346	4.24E-01	0.5026	0.084	8.64E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5477	4.19E-01	0.5050	0.065	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5614	4.17E-01	0.5007	0.065	1.11E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5750	4.14E-01	0.4960	0.064	1.11E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.5887	4.12E-01	0.4918	0.064	1.10E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6024	4.09E-01	0.4875	0.063	1.10E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000

Table 3–3. Methyl *tert*-butyl ether output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	Air
								Source Apportionment				
0.6160	4.07E-01	0.4833	0.062	1.10E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6297	4.04E-01	0.4790	0.062	1.09E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6433	4.01E-01	0.4743	0.061	1.09E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6570	3.99E-01	0.4702	0.061	1.08E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6707	3.96E-01	0.4659	0.060	1.08E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6843	3.94E-01	0.4615	0.060	1.07E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.6980	3.91E-01	0.4572	0.059	1.07E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7116	3.89E-01	0.4529	0.058	1.06E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7253	3.86E-01	0.4485	0.058	1.06E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7390	3.84E-01	0.4442	0.057	1.05E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7526	3.81E-01	0.4399	0.057	1.05E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7663	3.79E-01	0.4356	0.056	1.04E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7799	3.76E-01	0.4312	0.056	1.04E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.7936	3.74E-01	0.4269	0.055	1.03E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8073	3.71E-01	0.4225	0.055	1.03E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8209	3.69E-01	0.4182	0.054	1.02E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8346	3.66E-01	0.4139	0.053	1.02E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8482	3.64E-01	0.4096	0.053	1.01E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8619	3.62E-01	0.4052	0.052	1.01E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8756	3.59E-01	0.4009	0.052	1.00E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.8892	3.57E-01	0.3966	0.051	9.99E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9029	3.54E-01	0.3922	0.051	9.94E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9165	3.52E-01	0.3879	0.050	9.89E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9302	3.49E-01	0.3836	0.050	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9438	3.46E-01	0.3793	0.049	1.12E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9575	3.43E-01	0.3749	0.048	1.11E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9712	3.41E-01	0.3706	0.048	1.10E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9848	3.38E-01	0.3662	0.047	1.09E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
0.9985	3.35E-01	0.3619	0.047	1.08E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0121	3.33E-01	0.3576	0.046	1.07E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0258	3.30E-01	0.3532	0.046	1.06E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0395	3.27E-01	0.3489	0.045	1.06E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0531	3.25E-01	0.3446	0.045	1.05E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0668	3.22E-01	0.3403	0.044	1.04E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0804	3.19E-01	0.3359	0.043	1.03E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.0934	3.17E-01	0.3333	0.047	7.80E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1066	3.06E-01	0.3448	0.063	8.22E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1197	2.94E-01	0.3576	0.066	8.36E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1328	2.83E-01	0.3704	0.068	8.50E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1459	2.73E-01	0.3833	0.070	8.63E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1589	2.70E-01	0.3839	0.067	7.62E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1721	2.70E-01	0.3734	0.065	7.52E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1853	2.69E-01	0.3630	0.063	7.42E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.1984	2.69E-01	0.3526	0.061	7.32E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2116	2.68E-01	0.3421	0.059	7.21E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2247	2.68E-01	0.3317	0.058	7.11E-06	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000

Table 3–3. Methyl *tert*-butyl ether output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment					
							ID	1	2	3	4	Air
1.2377	2.67E-01	0.3273	0.246	1.94E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2512	2.67E-01	0.3265	0.245	1.94E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2647	2.66E-01	0.3256	0.245	1.94E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2782	2.65E-01	0.3247	0.244	1.93E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.2916	2.65E-01	0.3239	0.243	1.93E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3051	2.64E-01	0.3230	0.243	1.93E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3186	2.63E-01	0.3221	0.242	1.93E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3320	2.63E-01	0.3213	0.241	1.93E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3455	2.62E-01	0.3204	0.241	1.92E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3590	2.62E-01	0.3196	0.240	1.92E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3724	2.61E-01	0.3187	0.239	1.92E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3859	2.60E-01	0.3179	0.239	1.92E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.3994	2.60E-01	0.3170	0.238	1.91E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4128	2.59E-01	0.3162	0.237	1.91E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4263	2.58E-01	0.3153	0.237	1.91E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4398	2.58E-01	0.3144	0.236	1.91E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4533	2.57E-01	0.3136	0.235	1.91E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4667	2.57E-01	0.3127	0.235	1.90E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4802	2.56E-01	0.3118	0.234	1.90E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.4937	2.55E-01	0.3110	0.234	1.90E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5071	2.55E-01	0.3101	0.233	1.90E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5206	2.54E-01	0.3093	0.232	1.89E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5341	2.53E-01	0.3084	0.232	1.89E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5475	2.53E-01	0.3075	0.231	1.89E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5610	2.52E-01	0.3067	0.230	1.89E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5745	2.52E-01	0.3058	0.230	1.89E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.5879	2.51E-01	0.3049	0.229	1.88E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.6014	2.50E-01	0.3041	0.228	1.88E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.6149	2.50E-01	0.3032	0.228	1.88E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.6284	2.49E-01	0.3024	0.227	1.88E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.6418	2.49E-01	0.3015	0.226	1.87E-05	0.00E+00	4.45E-02	0	0.946	0.054	0.000	0.000	0.000
1.6551	1.79E+00	0.5036	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.6686	1.75E+00	0.5045	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.6821	1.71E+00	0.5050	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.6956	1.67E+00	0.5059	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7091	1.63E+00	0.5069	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7226	1.60E+00	0.5078	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7361	1.56E+00	0.5088	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7496	1.53E+00	0.5092	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7631	1.49E+00	0.5102	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7766	1.46E+00	0.5111	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.7902	1.43E+00	0.5121	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8037	1.40E+00	0.5130	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8172	1.37E+00	0.5139	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8307	1.34E+00	0.5144	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8442	1.31E+00	0.5154	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8577	1.28E+00	0.5163	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000

Table 3–3. Methyl *tert*-butyl ether output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment					
							ID	1	2	3	4	Air
1.8712	1.25E+00	0.5172	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8847	1.22E+00	0.5182	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.8977	1.20E+00	0.5187	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9112	1.19E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9247	1.19E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9382	1.19E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9517	1.19E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9652	1.18E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9788	1.18E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
1.9923	1.18E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0058	1.18E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0193	1.17E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0328	1.17E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0463	1.17E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0598	1.17E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0733	1.16E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.0868	1.16E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1003	1.16E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1138	1.16E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1274	1.15E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1409	1.15E+00	0.5187	0.026	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1541	1.14E+00	0.5191	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1672	1.12E+00	0.5201	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1803	1.10E+00	0.5210	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.1933	1.08E+00	0.5224	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2064	1.06E+00	0.5234	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2195	1.04E+00	0.5243	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2326	1.02E+00	0.5257	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2456	9.97E-01	0.5267	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2587	9.78E-01	0.5276	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2718	9.60E-01	0.5290	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2849	9.42E-01	0.5300	0.003	8.05E-06	0.00E+00	4.45E-02	0	0.078	0.004	0.918	0.000	0.000
2.2979	6.97E-01	0.5305	0.039	8.05E-06	1.36E-11	4.45E-02	4	0.078	0.004	0.917	0.001	0.000
2.3112	6.97E-01	0.5314	0.046	4.78E-06	1.19E-09	4.45E-02	4	0.078	0.004	0.913	0.005	0.000
2.3243	6.97E-01	0.5324	0.047	4.78E-06	1.19E-09	4.45E-02	4	0.077	0.004	0.910	0.008	0.000
2.3375	6.97E-01	0.5333	0.047	4.79E-06	1.19E-09	4.45E-02	4	0.077	0.004	0.907	0.011	0.000
2.3507	6.98E-01	0.5342	0.047	4.79E-06	1.19E-09	4.45E-02	4	0.077	0.004	0.904	0.015	0.000
2.3639	6.98E-01	0.5352	0.047	4.80E-06	1.19E-09	4.45E-02	4	0.077	0.004	0.901	0.018	0.000
2.3770	6.98E-01	0.5361	0.047	4.80E-06	1.19E-09	4.45E-02	4	0.076	0.004	0.898	0.021	0.000
2.3902	6.99E-01	0.5371	0.047	4.81E-06	1.19E-09	4.45E-02	4	0.076	0.004	0.895	0.025	0.000
2.4034	6.99E-01	0.5380	0.047	4.82E-06	1.19E-09	4.45E-02	4	0.076	0.004	0.892	0.028	0.000
2.4166	6.99E-01	0.5390	0.047	4.82E-06	1.19E-09	4.45E-02	4	0.076	0.004	0.889	0.031	0.000
2.4297	7.00E-01	0.5399	0.047	4.83E-06	1.19E-09	4.45E-02	4	0.075	0.004	0.886	0.034	0.000
2.4429	7.00E-01	0.5408	0.047	4.83E-06	1.19E-09	4.45E-02	4	0.075	0.004	0.883	0.038	0.000
2.4561	7.00E-01	0.5418	0.047	4.84E-06	1.19E-09	4.45E-02	4	0.075	0.004	0.880	0.041	0.000
2.4692	7.00E-01	0.5427	0.047	4.85E-06	1.19E-09	4.45E-02	4	0.075	0.004	0.877	0.044	0.000
2.4824	7.01E-01	0.5437	0.047	4.85E-06	1.19E-09	4.45E-02	4	0.074	0.004	0.874	0.047	0.000

Table 3–3. Methyl *tert*-butyl ether output data, source synoptic inputs.—Continued

x (km)	c_i (μg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (μg)	c_s (μg/L)	Source Apportionment					
							ID	1	2	3	4	Air
2.4956	7.01E-01	0.5446	0.048	4.86E-06	1.19E-09	4.45E-02	4	0.074	0.004	0.872	0.050	0.000
2.5088	7.01E-01	0.5456	0.048	4.86E-06	1.19E-09	4.45E-02	4	0.074	0.004	0.869	0.053	0.000
2.5219	7.02E-01	0.5465	0.048	4.87E-06	1.19E-09	4.45E-02	4	0.074	0.004	0.866	0.057	0.000
2.5351	7.02E-01	0.5475	0.048	4.88E-06	1.19E-09	4.45E-02	4	0.073	0.004	0.863	0.060	0.000
2.5483	7.02E-01	0.5484	0.048	4.88E-06	1.19E-09	4.45E-02	4	0.073	0.004	0.860	0.063	0.000
2.5615	7.02E-01	0.5493	0.048	4.89E-06	1.19E-09	4.45E-02	4	0.073	0.004	0.857	0.066	0.000
2.5746	7.03E-01	0.5503	0.048	4.89E-06	1.19E-09	4.45E-02	4	0.073	0.004	0.855	0.069	0.000
2.5878	7.03E-01	0.5512	0.048	4.90E-06	1.19E-09	4.45E-02	4	0.072	0.004	0.852	0.072	0.000
2.6010	7.03E-01	0.5522	0.048	4.90E-06	1.19E-09	4.45E-02	4	0.072	0.004	0.849	0.075	0.000
2.6142	7.03E-01	0.5531	0.048	4.91E-06	1.19E-09	4.45E-02	4	0.072	0.004	0.846	0.078	0.000
2.6273	7.04E-01	0.5541	0.048	4.92E-06	1.19E-09	4.45E-02	4	0.072	0.004	0.844	0.081	0.000
2.6405	7.04E-01	0.5550	0.048	4.92E-06	1.19E-09	4.45E-02	4	0.071	0.004	0.841	0.084	0.000
2.6537	7.04E-01	0.5559	0.049	4.93E-06	1.19E-09	4.45E-02	4	0.071	0.004	0.838	0.087	0.000
2.6668	7.04E-01	0.5569	0.049	4.93E-06	1.19E-09	4.45E-02	4	0.071	0.004	0.835	0.090	0.000
2.6800	7.05E-01	0.5578	0.049	4.94E-06	1.19E-09	4.45E-02	4	0.071	0.004	0.833	0.093	0.000
2.6932	7.05E-01	0.5588	0.049	4.95E-06	1.19E-09	4.45E-02	4	0.071	0.004	0.830	0.095	0.000
2.7064	7.05E-01	0.5597	0.049	4.95E-06	1.19E-09	4.45E-02	4	0.070	0.004	0.828	0.098	0.000
2.7195	7.05E-01	0.5607	0.049	4.96E-06	1.19E-09	4.45E-02	4	0.070	0.004	0.825	0.101	0.000
2.7327	7.06E-01	0.5616	0.049	4.96E-06	1.19E-09	4.45E-02	4	0.070	0.004	0.822	0.104	0.000
2.7457	6.17E-01	0.5654	0.112	1.07E-05	0.00E+00	4.45E-02	0	0.070	0.004	0.822	0.105	0.000
2.7589	6.06E-01	0.5748	0.114	1.08E-05	0.00E+00	4.45E-02	0	0.070	0.004	0.822	0.105	0.000
2.7721	5.95E-01	0.5847	0.116	1.09E-05	0.00E+00	4.45E-02	0	0.070	0.004	0.822	0.105	0.000
2.7852	5.84E-01	0.5942	0.118	1.10E-05	0.00E+00	4.45E-02	0	0.070	0.004	0.822	0.105	0.000
2.7984	5.74E-01	0.6036	0.119	1.10E-05	0.00E+00	4.45E-02	0	0.070	0.004	0.822	0.105	0.000

Table 3–4. Chloroform output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	Air
0.0000	1.17E-01	0.3542	0.215	2.57E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0132	1.15E-01	0.3593	0.218	2.59E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0265	1.13E-01	0.3643	0.221	2.61E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0397	1.10E-01	0.3694	0.224	2.62E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0529	1.08E-01	0.3745	0.227	2.64E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0662	1.06E-01	0.3796	0.230	2.66E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0794	1.05E-01	0.3847	0.233	2.68E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.0926	1.03E-01	0.3897	0.236	2.69E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1062	1.02E-01	0.3914	0.101	1.35E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1197	1.01E-01	0.3924	0.101	1.35E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1332	1.01E-01	0.3934	0.102	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1467	9.99E-02	0.3944	0.102	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1602	9.94E-02	0.3955	0.102	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1737	9.88E-02	0.3965	0.103	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.1872	9.82E-02	0.3975	0.103	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2007	9.76E-02	0.3986	0.103	1.36E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2142	9.70E-02	0.3995	0.103	1.37E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2276	9.65E-02	0.4006	0.104	1.37E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2411	9.59E-02	0.4016	0.104	1.37E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2546	9.54E-02	0.4026	0.104	1.37E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2681	9.48E-02	0.4037	0.104	1.37E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2816	9.43E-02	0.4047	0.105	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.2951	9.37E-02	0.4057	0.105	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3086	9.32E-02	0.4067	0.105	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3221	9.26E-02	0.4078	0.105	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3356	9.21E-02	0.4087	0.106	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3490	9.16E-02	0.4098	0.106	1.38E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3625	9.10E-02	0.4108	0.106	1.39E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3760	9.05E-02	0.4118	0.106	1.39E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.3895	9.00E-02	0.4129	0.107	1.39E-05	0.00E+00	1.72E-03	0	1.000	0.000	0.000	0.000
0.4025	9.43E-02	0.4136	0.084	1.12E-05	8.05E-11	1.72E-03	2	0.950	0.050	0.000	0.000
0.4158	1.17E-01	0.4213	0.070	9.46E-06	2.17E-09	1.72E-03	2	0.753	0.247	0.000	0.000
0.4290	1.37E-01	0.4303	0.072	9.56E-06	2.17E-09	1.72E-03	2	0.624	0.376	0.000	0.000
0.4422	1.57E-01	0.4393	0.073	9.66E-06	2.17E-09	1.72E-03	2	0.533	0.467	0.000	0.000
0.4554	1.76E-01	0.4484	0.075	9.75E-06	2.17E-09	1.72E-03	2	0.465	0.535	0.000	0.000
0.4686	1.94E-01	0.4575	0.076	9.85E-06	2.17E-09	1.72E-03	2	0.412	0.588	0.000	0.000
0.4818	2.12E-01	0.4665	0.078	9.95E-06	2.17E-09	1.72E-03	2	0.370	0.630	0.000	0.000
0.4950	2.29E-01	0.4757	0.079	1.00E-05	2.17E-09	1.72E-03	2	0.335	0.665	0.000	0.000
0.5082	2.45E-01	0.4847	0.081	1.01E-05	2.17E-09	1.72E-03	2	0.307	0.693	0.000	0.000
0.5214	2.60E-01	0.4937	0.082	1.02E-05	2.17E-09	1.72E-03	2	0.283	0.717	0.000	0.000
0.5346	2.75E-01	0.5026	0.084	1.03E-05	2.17E-09	1.72E-03	2	0.262	0.738	0.000	0.000
0.5477	2.80E-01	0.5050	0.065	1.36E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.5614	2.77E-01	0.5007	0.065	1.35E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.5750	2.75E-01	0.4960	0.064	1.34E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.5887	2.73E-01	0.4918	0.064	1.34E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6024	2.70E-01	0.4875	0.063	1.33E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000

Table 3–4. Chloroform output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
0.6160	2.68E-01	0.4833	0.062	1.33E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6297	2.66E-01	0.4790	0.062	1.32E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6433	2.64E-01	0.4743	0.061	1.32E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6570	2.61E-01	0.4702	0.061	1.31E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6707	2.59E-01	0.4659	0.060	1.30E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6843	2.57E-01	0.4615	0.060	1.30E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.6980	2.55E-01	0.4572	0.059	1.29E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7116	2.52E-01	0.4529	0.058	1.29E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7253	2.50E-01	0.4485	0.058	1.28E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7390	2.48E-01	0.4442	0.057	1.27E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7526	2.46E-01	0.4399	0.057	1.27E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7663	2.44E-01	0.4356	0.056	1.26E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7799	2.42E-01	0.4312	0.056	1.25E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.7936	2.39E-01	0.4269	0.055	1.25E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8073	2.37E-01	0.4225	0.055	1.24E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8209	2.35E-01	0.4182	0.054	1.24E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8346	2.33E-01	0.4139	0.053	1.23E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8482	2.31E-01	0.4096	0.053	1.22E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8619	2.29E-01	0.4052	0.052	1.22E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8756	2.27E-01	0.4009	0.052	1.21E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.8892	2.24E-01	0.3966	0.051	1.20E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9029	2.22E-01	0.3922	0.051	1.20E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9165	2.20E-01	0.3879	0.050	1.19E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9302	2.18E-01	0.3836	0.050	1.37E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9438	2.15E-01	0.3793	0.049	1.35E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9575	2.13E-01	0.3749	0.048	1.34E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9712	2.11E-01	0.3706	0.048	1.33E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9848	2.08E-01	0.3662	0.047	1.32E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
0.9985	2.06E-01	0.3619	0.047	1.31E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0121	2.04E-01	0.3576	0.046	1.30E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0258	2.02E-01	0.3532	0.046	1.29E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0395	1.99E-01	0.3489	0.045	1.28E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0531	1.97E-01	0.3446	0.045	1.26E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0668	1.95E-01	0.3403	0.044	1.25E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0804	1.93E-01	0.3359	0.043	1.24E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.0934	1.91E-01	0.3333	0.047	9.28E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1066	1.84E-01	0.3448	0.063	9.79E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1197	1.77E-01	0.3576	0.066	9.97E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1328	1.70E-01	0.3704	0.068	1.02E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1459	1.64E-01	0.3833	0.070	1.03E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1589	1.62E-01	0.3839	0.067	9.05E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1721	1.61E-01	0.3734	0.065	8.92E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1853	1.61E-01	0.3630	0.063	8.80E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.1984	1.61E-01	0.3526	0.061	8.67E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2116	1.60E-01	0.3421	0.059	8.55E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2247	1.60E-01	0.3317	0.058	8.42E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000

Table 3–4. Chloroform output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
1.2377	1.59E-01	0.3273	0.246	2.48E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2512	1.59E-01	0.3265	0.245	2.48E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2647	1.58E-01	0.3256	0.245	2.48E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2782	1.58E-01	0.3247	0.244	2.47E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.2916	1.57E-01	0.3239	0.243	2.47E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3051	1.57E-01	0.3230	0.243	2.47E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3186	1.56E-01	0.3221	0.242	2.46E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3320	1.55E-01	0.3213	0.241	2.46E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3455	1.55E-01	0.3204	0.241	2.46E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3590	1.54E-01	0.3196	0.240	2.45E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3724	1.54E-01	0.3187	0.239	2.45E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3859	1.53E-01	0.3179	0.239	2.45E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.3994	1.53E-01	0.3170	0.238	2.44E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4128	1.52E-01	0.3162	0.237	2.44E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4263	1.51E-01	0.3153	0.237	2.44E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4398	1.51E-01	0.3144	0.236	2.43E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4533	1.50E-01	0.3136	0.235	2.43E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4667	1.50E-01	0.3127	0.235	2.43E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4802	1.49E-01	0.3118	0.234	2.42E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.4937	1.49E-01	0.3110	0.234	2.42E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5071	1.48E-01	0.3101	0.233	2.42E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5206	1.48E-01	0.3093	0.232	2.41E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5341	1.47E-01	0.3084	0.232	2.41E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5475	1.46E-01	0.3075	0.231	2.41E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5610	1.46E-01	0.3067	0.230	2.41E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5745	1.45E-01	0.3058	0.230	2.40E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.5879	1.45E-01	0.3049	0.229	2.40E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6014	1.44E-01	0.3041	0.228	2.40E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6149	1.44E-01	0.3032	0.228	2.39E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6284	1.43E-01	0.3024	0.227	2.39E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6418	1.43E-01	0.3015	0.226	2.39E-05	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6551	8.42E-02	0.5036	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6686	8.20E-02	0.5045	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6821	7.98E-02	0.5050	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.6956	7.77E-02	0.5059	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7091	7.57E-02	0.5069	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7226	7.37E-02	0.5078	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7361	7.17E-02	0.5088	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7496	6.99E-02	0.5092	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7631	6.81E-02	0.5102	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7766	6.63E-02	0.5111	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.7902	6.46E-02	0.5121	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8037	6.29E-02	0.5130	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8172	6.13E-02	0.5139	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8307	5.97E-02	0.5144	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8442	5.82E-02	0.5154	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8577	5.67E-02	0.5163	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000

Table 3–4.   Chloroform output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
1.8712	5.52E-02	0.5172	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8847	5.38E-02	0.5182	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.8977	5.25E-02	0.5187	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9112	5.22E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9247	5.21E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9382	5.20E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9517	5.18E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9652	5.17E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9788	5.16E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
1.9923	5.15E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0058	5.13E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0193	5.12E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0328	5.11E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0463	5.10E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0598	5.09E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0733	5.07E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.0868	5.06E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1003	5.05E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1138	5.04E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1274	5.02E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1409	5.01E-02	0.5187	0.026	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1541	4.97E-02	0.5191	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1672	4.85E-02	0.5201	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1803	4.74E-02	0.5210	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.1933	4.63E-02	0.5224	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2064	4.53E-02	0.5234	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2195	4.43E-02	0.5243	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2326	4.33E-02	0.5257	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2456	4.23E-02	0.5267	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2587	4.14E-02	0.5276	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2718	4.05E-02	0.5290	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2849	3.96E-02	0.5300	0.003	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.2979	2.62E-02	0.5305	0.039	9.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3112	2.61E-02	0.5314	0.046	5.57E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3243	2.60E-02	0.5324	0.047	5.58E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3375	2.59E-02	0.5333	0.047	5.59E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3507	2.59E-02	0.5342	0.047	5.60E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3639	2.58E-02	0.5352	0.047	5.60E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3770	2.57E-02	0.5361	0.047	5.61E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.3902	2.56E-02	0.5371	0.047	5.62E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4034	2.55E-02	0.5380	0.047	5.62E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4166	2.55E-02	0.5390	0.047	5.63E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4297	2.54E-02	0.5399	0.047	5.64E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4429	2.53E-02	0.5408	0.047	5.65E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4561	2.52E-02	0.5418	0.047	5.65E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4692	2.51E-02	0.5427	0.047	5.66E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.4824	2.51E-02	0.5437	0.047	5.67E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000

Table 3–4.   Chloroform output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
2.4956	2.50E-02	0.5446	0.048	5.67E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5088	2.49E-02	0.5456	0.048	5.68E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5219	2.48E-02	0.5465	0.048	5.69E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5351	2.48E-02	0.5475	0.048	5.69E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5483	2.47E-02	0.5484	0.048	5.70E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5615	2.46E-02	0.5493	0.048	5.71E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5746	2.45E-02	0.5503	0.048	5.72E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.5878	2.45E-02	0.5512	0.048	5.72E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6010	2.44E-02	0.5522	0.048	5.73E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6142	2.43E-02	0.5531	0.048	5.74E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6273	2.42E-02	0.5541	0.048	5.74E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6405	2.42E-02	0.5550	0.048	5.75E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6537	2.41E-02	0.5559	0.049	5.76E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6668	2.40E-02	0.5569	0.049	5.77E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6800	2.39E-02	0.5578	0.049	5.77E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.6932	2.39E-02	0.5588	0.049	5.78E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.7064	2.38E-02	0.5597	0.049	5.79E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.7195	2.37E-02	0.5607	0.049	5.79E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.7327	2.37E-02	0.5616	0.049	5.80E-06	0.00E+00	1.72E-03	0	0.255	0.745	0.000	0.000
2.7457	2.39E-02	0.5654	0.112	1.30E-05	3.80E-10	1.72E-03	3	0.210	0.615	0.174	0.000
2.7589	2.93E-02	0.5748	0.114	1.31E-05	3.80E-10	1.72E-03	3	0.168	0.491	0.341	0.000
2.7721	3.46E-02	0.5847	0.116	1.32E-05	3.80E-10	1.72E-03	3	0.140	0.409	0.451	0.000
2.7852	3.96E-02	0.5942	0.118	1.33E-05	3.80E-10	1.72E-03	3	0.120	0.350	0.531	0.000
2.7984	4.46E-02	0.6036	0.119	1.34E-05	3.80E-10	1.72E-03	3	0.105	0.306	0.590	0.000

Table 3–5. 1,1-Dichloroethane output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
0.0000	3.81E-02	0.3542	0.215	2.58E-05	4.48E-10	0.00E+00	2	0.997	0.003	0.000	0.000
0.0132	4.41E-02	0.3593	0.218	2.59E-05	4.48E-10	0.00E+00	2	0.844	0.156	0.000	0.000
0.0265	5.00E-02	0.3643	0.221	2.61E-05	4.48E-10	0.00E+00	2	0.731	0.269	0.000	0.000
0.0397	5.56E-02	0.3694	0.224	2.63E-05	4.48E-10	0.00E+00	2	0.645	0.355	0.000	0.000
0.0529	6.11E-02	0.3745	0.227	2.65E-05	4.48E-10	0.00E+00	2	0.576	0.424	0.000	0.000
0.0662	6.63E-02	0.3796	0.230	2.67E-05	4.48E-10	0.00E+00	2	0.521	0.479	0.000	0.000
0.0794	7.14E-02	0.3847	0.233	2.68E-05	4.48E-10	0.00E+00	2	0.475	0.525	0.000	0.000
0.0926	7.64E-02	0.3897	0.236	2.70E-05	4.48E-10	0.00E+00	2	0.436	0.564	0.000	0.000
0.1062	7.72E-02	0.3914	0.101	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1197	7.68E-02	0.3924	0.101	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1332	7.63E-02	0.3934	0.102	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1467	7.58E-02	0.3944	0.102	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1602	7.54E-02	0.3955	0.102	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1737	7.49E-02	0.3965	0.103	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.1872	7.45E-02	0.3975	0.103	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2007	7.41E-02	0.3986	0.103	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2142	7.36E-02	0.3995	0.103	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2276	7.32E-02	0.4006	0.104	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2411	7.28E-02	0.4016	0.104	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2546	7.23E-02	0.4026	0.104	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2681	7.19E-02	0.4037	0.104	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2816	7.15E-02	0.4047	0.105	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.2951	7.11E-02	0.4057	0.105	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3086	7.07E-02	0.4067	0.105	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3221	7.02E-02	0.4078	0.105	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3356	6.98E-02	0.4087	0.106	1.37E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3490	6.94E-02	0.4098	0.106	1.38E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3625	6.90E-02	0.4108	0.106	1.38E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3760	6.86E-02	0.4118	0.106	1.38E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.3895	6.82E-02	0.4129	0.107	1.38E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4025	6.79E-02	0.4136	0.084	1.11E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4158	6.65E-02	0.4213	0.070	9.38E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4290	6.50E-02	0.4303	0.072	9.48E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4422	6.35E-02	0.4393	0.073	9.58E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4554	6.21E-02	0.4484	0.075	9.68E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4686	6.07E-02	0.4575	0.076	9.78E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4818	5.94E-02	0.4665	0.078	9.87E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.4950	5.81E-02	0.4757	0.079	9.97E-06	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5082	5.69E-02	0.4847	0.081	1.01E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5214	5.58E-02	0.4937	0.082	1.02E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5346	5.46E-02	0.5026	0.084	1.02E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5477	5.40E-02	0.5050	0.065	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5614	5.36E-02	0.5007	0.065	1.34E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5750	5.31E-02	0.4960	0.064	1.34E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.5887	5.27E-02	0.4918	0.064	1.33E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6024	5.23E-02	0.4875	0.063	1.33E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000

Table 3–5. 1,1-Dichloroethane output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
0.6160	5.18E-02	0.4833	0.062	1.32E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6297	5.14E-02	0.4790	0.062	1.31E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6433	5.09E-02	0.4743	0.061	1.31E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6570	5.05E-02	0.4702	0.061	1.30E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6707	5.01E-02	0.4659	0.060	1.30E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6843	4.96E-02	0.4615	0.060	1.29E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.6980	4.92E-02	0.4572	0.059	1.28E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7116	4.88E-02	0.4529	0.058	1.28E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7253	4.83E-02	0.4485	0.058	1.27E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7390	4.79E-02	0.4442	0.057	1.27E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7526	4.75E-02	0.4399	0.057	1.26E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7663	4.71E-02	0.4356	0.056	1.25E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7799	4.67E-02	0.4312	0.056	1.25E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.7936	4.62E-02	0.4269	0.055	1.24E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8073	4.58E-02	0.4225	0.055	1.23E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8209	4.54E-02	0.4182	0.054	1.23E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8346	4.50E-02	0.4139	0.053	1.22E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8482	4.46E-02	0.4096	0.053	1.22E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8619	4.42E-02	0.4052	0.052	1.21E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8756	4.38E-02	0.4009	0.052	1.20E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.8892	4.34E-02	0.3966	0.051	1.20E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9029	4.29E-02	0.3922	0.051	1.19E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9165	4.25E-02	0.3879	0.050	1.18E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9302	4.21E-02	0.3836	0.050	1.36E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9438	4.16E-02	0.3793	0.049	1.35E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9575	4.12E-02	0.3749	0.048	1.34E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9712	4.07E-02	0.3706	0.048	1.32E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9848	4.03E-02	0.3662	0.047	1.31E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
0.9985	3.98E-02	0.3619	0.047	1.30E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0121	3.94E-02	0.3576	0.046	1.29E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0258	3.89E-02	0.3532	0.046	1.28E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0395	3.85E-02	0.3489	0.045	1.27E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0531	3.81E-02	0.3446	0.045	1.26E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0668	3.76E-02	0.3403	0.044	1.25E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0804	3.72E-02	0.3359	0.043	1.23E-05	0.00E+00	0.00E+00	0	0.428	0.572	0.000	0.000
1.0934	3.79E-02	0.3333	0.047	9.20E-06	1.36E-11	0.00E+00	3	0.415	0.556	0.029	0.000
1.1066	4.07E-02	0.3448	0.063	9.72E-06	1.50E-10	0.00E+00	3	0.373	0.500	0.127	0.000
1.1197	4.30E-02	0.3576	0.066	9.90E-06	1.50E-10	0.00E+00	3	0.339	0.454	0.207	0.000
1.1328	4.52E-02	0.3704	0.068	1.01E-05	1.50E-10	0.00E+00	3	0.311	0.416	0.274	0.000
1.1459	4.72E-02	0.3833	0.070	1.02E-05	1.50E-10	0.00E+00	3	0.287	0.383	0.330	0.000
1.1589	4.77E-02	0.3839	0.067	8.97E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.1721	4.76E-02	0.3734	0.065	8.85E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.1853	4.75E-02	0.3630	0.063	8.73E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.1984	4.74E-02	0.3526	0.061	8.60E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2116	4.73E-02	0.3421	0.059	8.47E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2247	4.72E-02	0.3317	0.058	8.35E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000

Table 3–5.   1,1-Dichloroethane output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
1.2377	4.70E-02	0.3273	0.246	2.49E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2512	4.69E-02	0.3265	0.245	2.48E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2647	4.67E-02	0.3256	0.245	2.48E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2782	4.65E-02	0.3247	0.244	2.48E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.2916	4.64E-02	0.3239	0.243	2.47E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3051	4.62E-02	0.3230	0.243	2.47E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3186	4.60E-02	0.3221	0.242	2.47E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3320	4.58E-02	0.3213	0.241	2.46E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3455	4.57E-02	0.3204	0.241	2.46E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3590	4.55E-02	0.3196	0.240	2.46E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3724	4.53E-02	0.3187	0.239	2.45E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3859	4.52E-02	0.3179	0.239	2.45E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.3994	4.50E-02	0.3170	0.238	2.45E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4128	4.48E-02	0.3162	0.237	2.44E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4263	4.47E-02	0.3153	0.237	2.44E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4398	4.45E-02	0.3144	0.236	2.44E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4533	4.43E-02	0.3136	0.235	2.43E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4667	4.42E-02	0.3127	0.235	2.43E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4802	4.40E-02	0.3118	0.234	2.43E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.4937	4.38E-02	0.3110	0.234	2.42E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5071	4.37E-02	0.3101	0.233	2.42E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5206	4.35E-02	0.3093	0.232	2.42E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5341	4.33E-02	0.3084	0.232	2.41E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5475	4.32E-02	0.3075	0.231	2.41E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5610	4.30E-02	0.3067	0.230	2.41E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5745	4.28E-02	0.3058	0.230	2.40E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.5879	4.27E-02	0.3049	0.229	2.40E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6014	4.25E-02	0.3041	0.228	2.40E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6149	4.24E-02	0.3032	0.228	2.39E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6284	4.22E-02	0.3024	0.227	2.39E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6418	4.20E-02	0.3015	0.226	2.39E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6551	2.48E-02	0.5036	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6686	2.41E-02	0.5045	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6821	2.35E-02	0.5050	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.6956	2.29E-02	0.5059	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7091	2.23E-02	0.5069	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7226	2.17E-02	0.5078	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7361	2.11E-02	0.5088	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7496	2.05E-02	0.5092	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7631	2.00E-02	0.5102	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7766	1.95E-02	0.5111	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.7902	1.89E-02	0.5121	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8037	1.84E-02	0.5130	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8172	1.80E-02	0.5139	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8307	1.75E-02	0.5144	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8442	1.70E-02	0.5154	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8577	1.66E-02	0.5163	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000

Table 3–5. 1,1-Dichloroethane output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	Air
							**Source Apportionment**				
1.8712	1.62E-02	0.5172	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8847	1.57E-02	0.5182	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.8977	1.53E-02	0.5187	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9112	1.53E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9247	1.52E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9382	1.52E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9517	1.51E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9652	1.51E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9788	1.51E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
1.9923	1.50E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0058	1.50E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0193	1.50E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0328	1.49E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0463	1.49E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0598	1.48E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0733	1.48E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.0868	1.48E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1003	1.47E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1138	1.47E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1274	1.47E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1409	1.46E-02	0.5187	0.026	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1541	1.45E-02	0.5191	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1672	1.42E-02	0.5201	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1803	1.38E-02	0.5210	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.1933	1.35E-02	0.5224	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2064	1.32E-02	0.5234	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2195	1.29E-02	0.5243	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2326	1.26E-02	0.5257	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2456	1.23E-02	0.5267	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2587	1.20E-02	0.5276	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2718	1.17E-02	0.5290	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2849	1.15E-02	0.5300	0.003	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.2979	7.41E-03	0.5305	0.039	9.50E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3112	7.39E-03	0.5314	0.046	5.52E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3243	7.36E-03	0.5324	0.047	5.52E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3375	7.34E-03	0.5333	0.047	5.53E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3507	7.31E-03	0.5342	0.047	5.54E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3639	7.29E-03	0.5352	0.047	5.55E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3770	7.27E-03	0.5361	0.047	5.55E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.3902	7.24E-03	0.5371	0.047	5.56E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4034	7.22E-03	0.5380	0.047	5.57E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4166	7.20E-03	0.5390	0.047	5.57E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4297	7.18E-03	0.5399	0.047	5.58E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4429	7.15E-03	0.5408	0.047	5.59E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4561	7.13E-03	0.5418	0.047	5.60E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4692	7.11E-03	0.5427	0.047	5.60E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.4824	7.08E-03	0.5437	0.047	5.61E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000

Table 3–5. 1,1-Dichloroethane output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment				
							ID	1	2	3	Air
2.4956	7.06E-03	0.5446	0.048	5.62E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5088	7.04E-03	0.5456	0.048	5.62E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5219	7.02E-03	0.5465	0.048	5.63E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5351	7.00E-03	0.5475	0.048	5.64E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5483	6.97E-03	0.5484	0.048	5.64E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5615	6.95E-03	0.5493	0.048	5.65E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5746	6.93E-03	0.5503	0.048	5.66E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.5878	6.91E-03	0.5512	0.048	5.67E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6010	6.89E-03	0.5522	0.048	5.67E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6142	6.86E-03	0.5531	0.048	5.68E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6273	6.84E-03	0.5541	0.048	5.69E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6405	6.82E-03	0.5550	0.048	5.69E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6537	6.80E-03	0.5559	0.049	5.70E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6668	6.78E-03	0.5569	0.049	5.71E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6800	6.76E-03	0.5578	0.049	5.71E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.6932	6.74E-03	0.5588	0.049	5.72E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7064	6.72E-03	0.5597	0.049	5.73E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7195	6.69E-03	0.5607	0.049	5.74E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7327	6.67E-03	0.5616	0.049	5.74E-06	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7457	5.48E-03	0.5654	0.112	1.29E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7589	5.37E-03	0.5748	0.114	1.30E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7721	5.27E-03	0.5847	0.116	1.31E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7852	5.17E-03	0.5942	0.118	1.32E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000
2.7984	5.08E-03	0.6036	0.119	1.33E-05	0.00E+00	0.00E+00	0	0.280	0.375	0.346	0.000

Table 3–6.   *cis*-1,2-Dichloroethene output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
							Source Apportionment						
0.0000	3.02E-01	0.3542	0.215	2.65E-05	2.19E-10	0.00E+00	2	1.000	0.000	0.000	0.000	0.000	0.000
0.0132	2.99E-01	0.3593	0.218	2.67E-05	2.19E-10	0.00E+00	2	0.989	0.011	0.000	0.000	0.000	0.000
0.0265	2.97E-01	0.3643	0.221	2.69E-05	2.19E-10	0.00E+00	2	0.978	0.022	0.000	0.000	0.000	0.000
0.0397	2.94E-01	0.3694	0.224	2.70E-05	2.19E-10	0.00E+00	2	0.968	0.032	0.000	0.000	0.000	0.000
0.0529	2.92E-01	0.3745	0.227	2.72E-05	2.19E-10	0.00E+00	2	0.958	0.042	0.000	0.000	0.000	0.000
0.0662	2.90E-01	0.3796	0.230	2.74E-05	2.19E-10	0.00E+00	2	0.947	0.053	0.000	0.000	0.000	0.000
0.0794	2.87E-01	0.3847	0.233	2.76E-05	2.19E-10	0.00E+00	2	0.937	0.063	0.000	0.000	0.000	0.000
0.0926	2.85E-01	0.3897	0.236	2.77E-05	2.19E-10	0.00E+00	2	0.928	0.072	0.000	0.000	0.000	0.000
0.1062	2.83E-01	0.3914	0.101	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1197	2.82E-01	0.3924	0.101	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1332	2.80E-01	0.3934	0.102	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1467	2.78E-01	0.3944	0.102	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1602	2.77E-01	0.3955	0.102	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1737	2.75E-01	0.3965	0.103	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.1872	2.73E-01	0.3975	0.103	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2007	2.72E-01	0.3986	0.103	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2142	2.70E-01	0.3995	0.103	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2276	2.68E-01	0.4006	0.104	1.41E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2411	2.67E-01	0.4016	0.104	1.41E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2546	2.65E-01	0.4026	0.104	1.41E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2681	2.64E-01	0.4037	0.104	1.41E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2816	2.62E-01	0.4047	0.105	1.41E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.2951	2.60E-01	0.4057	0.105	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3086	2.59E-01	0.4067	0.105	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3221	2.57E-01	0.4078	0.105	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3356	2.56E-01	0.4087	0.106	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3490	2.54E-01	0.4098	0.106	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3625	2.53E-01	0.4108	0.106	1.42E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3760	2.51E-01	0.4118	0.106	1.43E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.3895	2.50E-01	0.4129	0.107	1.43E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4025	2.49E-01	0.4136	0.084	1.15E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4158	2.43E-01	0.4213	0.070	9.72E-06	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4290	2.38E-01	0.4303	0.072	9.82E-06	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4422	2.32E-01	0.4393	0.073	9.92E-06	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4554	2.27E-01	0.4484	0.075	1.00E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4686	2.22E-01	0.4575	0.076	1.01E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4818	2.17E-01	0.4665	0.078	1.02E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.4950	2.13E-01	0.4757	0.079	1.03E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5082	2.08E-01	0.4847	0.081	1.04E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5214	2.04E-01	0.4937	0.082	1.05E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5346	2.00E-01	0.5026	0.084	1.06E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5477	1.98E-01	0.5050	0.065	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5614	1.96E-01	0.5007	0.065	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5750	1.94E-01	0.4960	0.064	1.38E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.5887	1.93E-01	0.4918	0.064	1.38E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6024	1.91E-01	0.4875	0.063	1.37E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000

Table 3–6. *cis*-1,2-Dichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	*Q* (m³/s)	*V* (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
										Source Apportionment			
0.6160	1.89E-01	0.4833	0.062	1.36E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6297	1.88E-01	0.4790	0.062	1.36E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6433	1.86E-01	0.4743	0.061	1.35E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6570	1.84E-01	0.4702	0.061	1.35E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6707	1.83E-01	0.4659	0.060	1.34E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6843	1.81E-01	0.4615	0.060	1.33E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.6980	1.79E-01	0.4572	0.059	1.33E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7116	1.78E-01	0.4529	0.058	1.32E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7253	1.76E-01	0.4485	0.058	1.32E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7390	1.75E-01	0.4442	0.057	1.31E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7526	1.73E-01	0.4399	0.057	1.30E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7663	1.71E-01	0.4356	0.056	1.30E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7799	1.70E-01	0.4312	0.056	1.29E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.7936	1.68E-01	0.4269	0.055	1.28E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8073	1.67E-01	0.4225	0.055	1.28E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8209	1.65E-01	0.4182	0.054	1.27E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8346	1.64E-01	0.4139	0.053	1.26E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8482	1.62E-01	0.4096	0.053	1.26E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8619	1.60E-01	0.4052	0.052	1.25E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8756	1.59E-01	0.4009	0.052	1.24E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.8892	1.57E-01	0.3966	0.051	1.24E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9029	1.56E-01	0.3922	0.051	1.23E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9165	1.54E-01	0.3879	0.050	1.22E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9302	1.53E-01	0.3836	0.050	1.40E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9438	1.51E-01	0.3793	0.049	1.39E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9575	1.49E-01	0.3749	0.048	1.38E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9712	1.47E-01	0.3706	0.048	1.37E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9848	1.46E-01	0.3662	0.047	1.36E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
0.9985	1.44E-01	0.3619	0.047	1.35E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0121	1.42E-01	0.3576	0.046	1.33E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0258	1.41E-01	0.3532	0.046	1.32E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0395	1.39E-01	0.3489	0.045	1.31E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0531	1.38E-01	0.3446	0.045	1.30E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0668	1.36E-01	0.3403	0.044	1.29E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0804	1.34E-01	0.3359	0.043	1.28E-05	0.00E+00	0.00E+00	0	0.925	0.075	0.000	0.000	0.000	0.000
1.0934	1.34E-01	0.3333	0.047	9.53E-06	1.39E-11	0.00E+00	3	0.918	0.074	0.008	0.000	0.000	0.000
1.1066	1.33E-01	0.3448	0.063	1.01E-05	1.53E-10	0.00E+00	3	0.889	0.072	0.039	0.000	0.000	0.000
1.1197	1.32E-01	0.3576	0.066	1.02E-05	1.53E-10	0.00E+00	3	0.863	0.070	0.067	0.000	0.000	0.000
1.1328	1.31E-01	0.3704	0.068	1.04E-05	1.53E-10	0.00E+00	3	0.838	0.068	0.095	0.000	0.000	0.000
1.1459	1.30E-01	0.3833	0.070	1.06E-05	1.53E-10	0.00E+00	3	0.814	0.066	0.120	0.000	0.000	0.000
1.1589	1.29E-01	0.3839	0.067	9.29E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.1721	1.29E-01	0.3734	0.065	9.17E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.1853	1.29E-01	0.3630	0.063	9.04E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.1984	1.28E-01	0.3526	0.061	8.91E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2116	1.28E-01	0.3421	0.059	8.78E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2247	1.28E-01	0.3317	0.058	8.65E-06	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2377	1.27E-01	0.3273	0.246	2.56E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000

Table 3–6. *cis*-1,2-Dichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment						
							ID	1	2	3	4	5	Air
1.2512	1.27E-01	0.3265	0.245	2.55E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2647	1.26E-01	0.3256	0.245	2.55E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2782	1.26E-01	0.3247	0.244	2.55E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.2916	1.25E-01	0.3239	0.243	2.54E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3051	1.25E-01	0.3230	0.243	2.54E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3186	1.24E-01	0.3221	0.242	2.54E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3320	1.24E-01	0.3213	0.241	2.53E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3455	1.23E-01	0.3204	0.241	2.53E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3590	1.23E-01	0.3196	0.240	2.53E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3724	1.23E-01	0.3187	0.239	2.52E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3859	1.22E-01	0.3179	0.239	2.52E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.3994	1.22E-01	0.3170	0.238	2.52E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4128	1.21E-01	0.3162	0.237	2.51E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4263	1.21E-01	0.3153	0.237	2.51E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4398	1.20E-01	0.3144	0.236	2.51E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4533	1.20E-01	0.3136	0.235	2.50E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4667	1.19E-01	0.3127	0.235	2.50E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4802	1.19E-01	0.3118	0.234	2.50E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.4937	1.18E-01	0.3110	0.234	2.49E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5071	1.18E-01	0.3101	0.233	2.49E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5206	1.17E-01	0.3093	0.232	2.49E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5341	1.17E-01	0.3084	0.232	2.48E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5475	1.17E-01	0.3075	0.231	2.48E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5610	1.16E-01	0.3067	0.230	2.48E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5745	1.16E-01	0.3058	0.230	2.47E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.5879	1.15E-01	0.3049	0.229	2.47E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.6014	1.15E-01	0.3041	0.228	2.47E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.6149	1.14E-01	0.3032	0.228	2.46E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.6284	1.14E-01	0.3024	0.227	2.46E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.6418	1.13E-01	0.3015	0.226	2.46E-05	0.00E+00	0.00E+00	0	0.807	0.065	0.128	0.000	0.000	0.000
1.6551	7.96E-02	0.5036	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.6686	7.74E-02	0.5045	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.6821	7.52E-02	0.5050	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.6956	7.31E-02	0.5059	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7091	7.11E-02	0.5069	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7226	6.92E-02	0.5078	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7361	6.73E-02	0.5088	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7496	6.54E-02	0.5092	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7631	6.36E-02	0.5102	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7766	6.19E-02	0.5111	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.7902	6.02E-02	0.5121	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8037	5.86E-02	0.5130	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8172	5.70E-02	0.5139	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8307	5.54E-02	0.5144	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8442	5.39E-02	0.5154	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8577	5.25E-02	0.5163	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8712	5.11E-02	0.5172	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000

Table 3–6. *cis*-1,2-Dichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
										Source Apportionment			
1.8847	4.97E-02	0.5182	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.8977	4.84E-02	0.5187	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9112	4.81E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9247	4.80E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9382	4.79E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9517	4.78E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9652	4.76E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9788	4.75E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
1.9923	4.74E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0058	4.73E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0193	4.72E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0328	4.70E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0463	4.69E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0598	4.68E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0733	4.67E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.0868	4.66E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1003	4.64E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1138	4.63E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1274	4.62E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1409	4.61E-02	0.5187	0.026	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1541	4.56E-02	0.5191	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1672	4.45E-02	0.5201	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1803	4.35E-02	0.5210	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.1933	4.24E-02	0.5224	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2064	4.14E-02	0.5234	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2195	4.04E-02	0.5243	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2326	3.95E-02	0.5257	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2456	3.85E-02	0.5267	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2587	3.76E-02	0.5276	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2718	3.67E-02	0.5290	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2849	3.58E-02	0.5300	0.003	9.84E-06	0.00E+00	0.00E+00	0	0.678	0.055	0.107	0.160	0.000	0.000
2.2979	2.31E-02	0.5305	0.039	9.84E-06	3.00E-12	0.00E+00	5	0.672	0.054	0.106	0.158	0.009	0.000
2.3112	2.36E-02	0.5314	0.046	5.72E-06	2.63E-10	0.00E+00	5	0.656	0.053	0.104	0.154	0.034	0.000
2.3243	2.41E-02	0.5324	0.047	5.73E-06	2.63E-10	0.00E+00	5	0.640	0.052	0.101	0.151	0.057	0.000
2.3375	2.46E-02	0.5333	0.047	5.74E-06	2.63E-10	0.00E+00	5	0.625	0.051	0.099	0.147	0.079	0.000
2.3507	2.51E-02	0.5342	0.047	5.74E-06	2.63E-10	0.00E+00	5	0.611	0.049	0.097	0.144	0.100	0.000
2.3639	2.56E-02	0.5352	0.047	5.75E-06	2.63E-10	0.00E+00	5	0.597	0.048	0.095	0.141	0.120	0.000
2.3770	2.61E-02	0.5361	0.047	5.76E-06	2.63E-10	0.00E+00	5	0.584	0.047	0.092	0.138	0.139	0.000
2.3902	2.66E-02	0.5371	0.047	5.77E-06	2.63E-10	0.00E+00	5	0.572	0.046	0.090	0.135	0.157	0.000
2.4034	2.70E-02	0.5380	0.047	5.77E-06	2.63E-10	0.00E+00	5	0.560	0.045	0.089	0.132	0.175	0.000
2.4166	2.75E-02	0.5390	0.047	5.78E-06	2.63E-10	0.00E+00	5	0.548	0.044	0.087	0.129	0.192	0.000
2.4297	2.80E-02	0.5399	0.047	5.79E-06	2.63E-10	0.00E+00	5	0.537	0.043	0.085	0.127	0.208	0.000
2.4429	2.85E-02	0.5408	0.047	5.80E-06	2.63E-10	0.00E+00	5	0.526	0.043	0.083	0.124	0.224	0.000
2.4561	2.89E-02	0.5418	0.047	5.80E-06	2.63E-10	0.00E+00	5	0.516	0.042	0.082	0.122	0.239	0.000
2.4692	2.94E-02	0.5427	0.047	5.81E-06	2.63E-10	0.00E+00	5	0.506	0.041	0.080	0.119	0.254	0.000
2.4824	2.99E-02	0.5437	0.047	5.82E-06	2.63E-10	0.00E+00	5	0.497	0.040	0.079	0.117	0.268	0.000
2.4956	3.03E-02	0.5446	0.048	5.82E-06	2.63E-10	0.00E+00	5	0.488	0.039	0.077	0.115	0.281	0.000

Table 3–6. *cis*-1,2-Dichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	ID	1	2	3	4	5	Air
2.5088	3.08E-02	0.5456	0.048	5.83E-06	2.63E-10	0.00E+00	5	0.479	0.039	0.076	0.113	0.294	0.000
2.5219	3.13E-02	0.5465	0.048	5.84E-06	2.63E-10	0.00E+00	5	0.470	0.038	0.074	0.111	0.307	0.000
2.5351	3.17E-02	0.5475	0.048	5.85E-06	2.63E-10	0.00E+00	5	0.462	0.037	0.073	0.109	0.319	0.000
2.5483	3.22E-02	0.5484	0.048	5.85E-06	2.63E-10	0.00E+00	5	0.454	0.037	0.072	0.107	0.331	0.000
2.5615	3.26E-02	0.5493	0.048	5.86E-06	2.63E-10	0.00E+00	5	0.446	0.036	0.071	0.105	0.342	0.000
2.5746	3.31E-02	0.5503	0.048	5.87E-06	2.63E-10	0.00E+00	5	0.439	0.035	0.069	0.103	0.353	0.000
2.5878	3.35E-02	0.5512	0.048	5.88E-06	2.63E-10	0.00E+00	5	0.431	0.035	0.068	0.102	0.364	0.000
2.6010	3.40E-02	0.5522	0.048	5.88E-06	2.63E-10	0.00E+00	5	0.424	0.034	0.067	0.100	0.374	0.000
2.6142	3.44E-02	0.5531	0.048	5.89E-06	2.63E-10	0.00E+00	5	0.418	0.034	0.066	0.098	0.384	0.000
2.6273	3.49E-02	0.5541	0.048	5.90E-06	2.63E-10	0.00E+00	5	0.411	0.033	0.065	0.097	0.394	0.000
2.6405	3.53E-02	0.5550	0.048	5.90E-06	2.63E-10	0.00E+00	5	0.405	0.033	0.064	0.095	0.404	0.000
2.6537	3.57E-02	0.5559	0.049	5.91E-06	2.63E-10	0.00E+00	5	0.398	0.032	0.063	0.094	0.413	0.000
2.6668	3.62E-02	0.5569	0.049	5.92E-06	2.63E-10	0.00E+00	5	0.392	0.032	0.062	0.092	0.422	0.000
2.6800	3.66E-02	0.5578	0.049	5.93E-06	2.63E-10	0.00E+00	5	0.386	0.031	0.061	0.091	0.430	0.000
2.6932	3.70E-02	0.5588	0.049	5.93E-06	2.63E-10	0.00E+00	5	0.381	0.031	0.060	0.090	0.439	0.000
2.7064	3.75E-02	0.5597	0.049	5.94E-06	2.63E-10	0.00E+00	5	0.375	0.030	0.059	0.088	0.447	0.000
2.7195	3.79E-02	0.5607	0.049	5.95E-06	2.63E-10	0.00E+00	5	0.370	0.030	0.059	0.087	0.455	0.000
2.7327	3.83E-02	0.5616	0.049	5.95E-06	2.63E-10	0.00E+00	5	0.365	0.029	0.058	0.086	0.463	0.000
2.7457	3.14E-02	0.5654	0.112	1.33E-05	0.00E+00	0.00E+00	0	0.364	0.029	0.058	0.086	0.464	0.000
2.7589	3.08E-02	0.5748	0.114	1.34E-05	0.00E+00	0.00E+00	0	0.364	0.029	0.058	0.086	0.464	0.000
2.7721	3.02E-02	0.5847	0.116	1.35E-05	0.00E+00	0.00E+00	0	0.364	0.029	0.058	0.086	0.464	0.000
2.7852	2.96E-02	0.5942	0.118	1.36E-05	0.00E+00	0.00E+00	0	0.364	0.029	0.058	0.086	0.464	0.000
2.7984	2.91E-02	0.6036	0.119	1.38E-05	0.00E+00	0.00E+00	0	0.364	0.029	0.058	0.086	0.464	0.000

Table 3–7.   Trichloroethene output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment ID	1	2	3	4	5	Air
0.0000	1.74E-01	0.3542	0.215	2.55E-05	1.48E-10	1.96E-04	2	1.000	0.000	0.000	0.000	0.000	0.000
0.0132	1.74E-01	0.3593	0.218	2.57E-05	1.48E-10	1.96E-04	2	0.983	0.017	0.000	0.000	0.000	0.000
0.0265	1.73E-01	0.3643	0.221	2.59E-05	1.48E-10	1.96E-04	2	0.966	0.034	0.000	0.000	0.000	0.000
0.0397	1.73E-01	0.3694	0.224	2.61E-05	1.48E-10	1.96E-04	2	0.950	0.050	0.000	0.000	0.000	0.000
0.0529	1.73E-01	0.3745	0.227	2.63E-05	1.48E-10	1.96E-04	2	0.934	0.066	0.000	0.000	0.000	0.000
0.0662	1.72E-01	0.3796	0.230	2.64E-05	1.48E-10	1.96E-04	2	0.919	0.081	0.000	0.000	0.000	0.000
0.0794	1.72E-01	0.3847	0.233	2.66E-05	1.48E-10	1.96E-04	2	0.904	0.096	0.000	0.000	0.000	0.000
0.0926	1.71E-01	0.3897	0.236	2.68E-05	1.48E-10	1.96E-04	2	0.890	0.110	0.000	0.000	0.000	0.000
0.1062	1.71E-01	0.3914	0.101	1.33E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1197	1.70E-01	0.3924	0.101	1.33E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1332	1.69E-01	0.3934	0.102	1.33E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1467	1.68E-01	0.3944	0.102	1.33E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1602	1.67E-01	0.3955	0.102	1.33E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1737	1.66E-01	0.3965	0.103	1.34E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.1872	1.65E-01	0.3975	0.103	1.34E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2007	1.64E-01	0.3986	0.103	1.34E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2142	1.63E-01	0.3995	0.103	1.34E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2276	1.62E-01	0.4006	0.104	1.34E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2411	1.61E-01	0.4016	0.104	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2546	1.60E-01	0.4026	0.104	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2681	1.59E-01	0.4037	0.104	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2816	1.58E-01	0.4047	0.105	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.2951	1.57E-01	0.4057	0.105	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3086	1.56E-01	0.4067	0.105	1.35E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3221	1.55E-01	0.4078	0.105	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3356	1.54E-01	0.4087	0.106	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3490	1.54E-01	0.4098	0.106	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3625	1.53E-01	0.4108	0.106	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3760	1.52E-01	0.4118	0.106	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.3895	1.51E-01	0.4129	0.107	1.36E-05	0.00E+00	1.96E-04	0	0.887	0.113	0.000	0.000	0.000	0.000
0.4025	1.52E-01	0.4136	0.084	1.10E-05	2.46E-11	1.96E-04	3	0.877	0.112	0.010	0.000	0.000	0.000
0.4158	1.57E-01	0.4213	0.070	9.25E-06	6.64E-10	1.96E-04	3	0.832	0.106	0.062	0.000	0.000	0.000
0.4290	1.61E-01	0.4303	0.072	9.35E-06	6.64E-10	1.96E-04	3	0.791	0.101	0.108	0.000	0.000	0.000
0.4422	1.65E-01	0.4393	0.073	9.45E-06	6.64E-10	1.96E-04	3	0.754	0.096	0.150	0.000	0.000	0.000
0.4554	1.69E-01	0.4484	0.075	9.54E-06	6.64E-10	1.96E-04	3	0.720	0.092	0.188	0.000	0.000	0.000
0.4686	1.73E-01	0.4575	0.076	9.64E-06	6.64E-10	1.96E-04	3	0.689	0.088	0.223	0.000	0.000	0.000
0.4818	1.76E-01	0.4665	0.078	9.73E-06	6.64E-10	1.96E-04	3	0.661	0.085	0.255	0.000	0.000	0.000
0.4950	1.80E-01	0.4757	0.079	9.83E-06	6.64E-10	1.96E-04	3	0.635	0.081	0.284	0.000	0.000	0.000
0.5082	1.83E-01	0.4847	0.081	9.92E-06	6.64E-10	1.96E-04	3	0.610	0.078	0.312	0.000	0.000	0.000
0.5214	1.86E-01	0.4937	0.082	1.00E-05	6.64E-10	1.96E-04	3	0.588	0.075	0.337	0.000	0.000	0.000
0.5346	1.89E-01	0.5026	0.084	1.01E-05	6.64E-10	1.96E-04	3	0.567	0.072	0.361	0.000	0.000	0.000
0.5477	1.90E-01	0.5050	0.065	1.33E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.5614	1.88E-01	0.5007	0.065	1.33E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.5750	1.87E-01	0.4960	0.064	1.32E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.5887	1.85E-01	0.4918	0.064	1.31E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6024	1.84E-01	0.4875	0.063	1.31E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000

Table 3–7. Trichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment						
							ID	1	2	3	4	5	Air
0.6160	1.82E-01	0.4833	0.062	1.30E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6297	1.80E-01	0.4790	0.062	1.30E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6433	1.79E-01	0.4743	0.061	1.29E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6570	1.77E-01	0.4702	0.061	1.28E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6707	1.76E-01	0.4659	0.060	1.28E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6843	1.74E-01	0.4615	0.060	1.27E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.6980	1.73E-01	0.4572	0.059	1.27E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7116	1.71E-01	0.4529	0.058	1.26E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7253	1.70E-01	0.4485	0.058	1.26E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7390	1.69E-01	0.4442	0.057	1.25E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7526	1.67E-01	0.4399	0.057	1.24E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7663	1.66E-01	0.4356	0.056	1.24E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7799	1.64E-01	0.4312	0.056	1.23E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.7936	1.63E-01	0.4269	0.055	1.22E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8073	1.61E-01	0.4225	0.055	1.22E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8209	1.60E-01	0.4182	0.054	1.21E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8346	1.58E-01	0.4139	0.053	1.21E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8482	1.57E-01	0.4096	0.053	1.20E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8619	1.55E-01	0.4052	0.052	1.19E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8756	1.54E-01	0.4009	0.052	1.19E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.8892	1.53E-01	0.3966	0.051	1.18E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9029	1.51E-01	0.3922	0.051	1.17E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9165	1.50E-01	0.3879	0.050	1.17E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9302	1.48E-01	0.3836	0.050	1.34E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9438	1.47E-01	0.3793	0.049	1.33E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9575	1.45E-01	0.3749	0.048	1.32E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9712	1.43E-01	0.3706	0.048	1.31E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9848	1.42E-01	0.3662	0.047	1.30E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
0.9985	1.40E-01	0.3619	0.047	1.29E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0121	1.39E-01	0.3576	0.046	1.27E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0258	1.37E-01	0.3532	0.046	1.26E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0395	1.36E-01	0.3489	0.045	1.25E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0531	1.34E-01	0.3446	0.045	1.24E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0668	1.33E-01	0.3403	0.044	1.23E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0804	1.31E-01	0.3359	0.043	1.22E-05	0.00E+00	1.96E-04	0	0.559	0.072	0.370	0.000	0.000	0.000
1.0934	1.40E-01	0.3333	0.047	9.07E-06	9.33E-11	1.96E-04	4	0.519	0.066	0.343	0.072	0.000	0.000
1.1066	1.72E-01	0.3448	0.063	9.58E-06	1.03E-09	1.96E-04	4	0.407	0.052	0.269	0.273	0.000	0.000
1.1197	2.01E-01	0.3576	0.066	9.76E-06	1.03E-09	1.96E-04	4	0.334	0.043	0.221	0.402	0.000	0.000
1.1328	2.28E-01	0.3704	0.068	9.93E-06	1.03E-09	1.96E-04	4	0.284	0.036	0.188	0.492	0.000	0.000
1.1459	2.53E-01	0.3833	0.070	1.01E-05	1.03E-09	1.96E-04	4	0.247	0.032	0.163	0.559	0.000	0.000
1.1589	2.60E-01	0.3839	0.067	8.84E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.1721	2.60E-01	0.3734	0.065	8.72E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.1853	2.59E-01	0.3630	0.063	8.60E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.1984	2.58E-01	0.3526	0.061	8.48E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2116	2.58E-01	0.3421	0.059	8.35E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2247	2.57E-01	0.3317	0.058	8.22E-06	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000

Table 3–7. Trichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment						
							ID	1	2	3	4	5	Air
1.2377	2.56E-01	0.3273	0.246	2.46E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2512	2.56E-01	0.3265	0.245	2.46E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2647	2.55E-01	0.3256	0.245	2.46E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2782	2.54E-01	0.3247	0.244	2.45E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.2916	2.53E-01	0.3239	0.243	2.45E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3051	2.52E-01	0.3230	0.243	2.45E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3186	2.51E-01	0.3221	0.242	2.44E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3320	2.50E-01	0.3213	0.241	2.44E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3455	2.49E-01	0.3204	0.241	2.44E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3590	2.48E-01	0.3196	0.240	2.43E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3724	2.47E-01	0.3187	0.239	2.43E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3859	2.46E-01	0.3179	0.239	2.43E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.3994	2.45E-01	0.3170	0.238	2.42E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4128	2.45E-01	0.3162	0.237	2.42E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4263	2.44E-01	0.3153	0.237	2.42E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4398	2.43E-01	0.3144	0.236	2.41E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4533	2.42E-01	0.3136	0.235	2.41E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4667	2.41E-01	0.3127	0.235	2.41E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4802	2.40E-01	0.3118	0.234	2.40E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.4937	2.39E-01	0.3110	0.234	2.40E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5071	2.38E-01	0.3101	0.233	2.40E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5206	2.37E-01	0.3093	0.232	2.40E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5341	2.36E-01	0.3084	0.232	2.39E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5475	2.36E-01	0.3075	0.231	2.39E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5610	2.35E-01	0.3067	0.230	2.39E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5745	2.34E-01	0.3058	0.230	2.38E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.5879	2.33E-01	0.3049	0.229	2.38E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.6014	2.32E-01	0.3041	0.228	2.38E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.6149	2.31E-01	0.3032	0.228	2.37E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.6284	2.30E-01	0.3024	0.227	2.37E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.6418	2.29E-01	0.3015	0.226	2.37E-05	0.00E+00	1.96E-04	0	0.237	0.030	0.157	0.576	0.000	0.000
1.6551	1.49E-01	0.5036	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.6686	1.45E-01	0.5045	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.6821	1.42E-01	0.5050	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.6956	1.38E-01	0.5059	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7091	1.34E-01	0.5069	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7226	1.31E-01	0.5078	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7361	1.27E-01	0.5088	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7496	1.24E-01	0.5092	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7631	1.21E-01	0.5102	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7766	1.18E-01	0.5111	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.7902	1.15E-01	0.5121	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8037	1.12E-01	0.5130	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8172	1.09E-01	0.5139	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8307	1.06E-01	0.5144	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8442	1.03E-01	0.5154	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8577	1.00E-01	0.5163	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000

Table 3–7. Trichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment						
							ID	1	2	3	4	5	Air
1.8712	9.78E-02	0.5172	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8847	9.53E-02	0.5182	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.8977	9.30E-02	0.5187	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9112	9.25E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9247	9.22E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9382	9.20E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9517	9.18E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9652	9.16E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9788	9.14E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
1.9923	9.11E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0058	9.09E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0193	9.07E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0328	9.05E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0463	9.02E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0598	9.00E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0733	8.98E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.0868	8.96E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1003	8.94E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1138	8.92E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1274	8.89E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1409	8.87E-02	0.5187	0.026	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1541	8.79E-02	0.5191	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1672	8.59E-02	0.5201	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1803	8.39E-02	0.5210	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.1933	8.20E-02	0.5224	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2064	8.01E-02	0.5234	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2195	7.83E-02	0.5243	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2326	7.65E-02	0.5257	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2456	7.48E-02	0.5267	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2587	7.31E-02	0.5276	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2718	7.14E-02	0.5290	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2849	6.98E-02	0.5300	0.003	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.2979	4.53E-02	0.5305	0.039	9.37E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3112	4.51E-02	0.5314	0.046	5.43E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3243	4.50E-02	0.5324	0.047	5.44E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3375	4.49E-02	0.5333	0.047	5.44E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3507	4.47E-02	0.5342	0.047	5.45E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3639	4.46E-02	0.5352	0.047	5.46E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3770	4.44E-02	0.5361	0.047	5.47E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.3902	4.43E-02	0.5371	0.047	5.47E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4034	4.41E-02	0.5380	0.047	5.48E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4166	4.40E-02	0.5390	0.047	5.49E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4297	4.39E-02	0.5399	0.047	5.49E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4429	4.37E-02	0.5408	0.047	5.50E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4561	4.36E-02	0.5418	0.047	5.51E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4692	4.35E-02	0.5427	0.047	5.51E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.4824	4.33E-02	0.5437	0.047	5.52E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000

Table 3–7. Trichloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment						
							ID	1	2	3	4	5	Air
2.4956	4.32E-02	0.5446	0.048	5.53E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5088	4.30E-02	0.5456	0.048	5.54E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5219	4.29E-02	0.5465	0.048	5.54E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5351	4.28E-02	0.5475	0.048	5.55E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5483	4.26E-02	0.5484	0.048	5.56E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5615	4.25E-02	0.5493	0.048	5.56E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5746	4.24E-02	0.5503	0.048	5.57E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.5878	4.22E-02	0.5512	0.048	5.58E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6010	4.21E-02	0.5522	0.048	5.58E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6142	4.20E-02	0.5531	0.048	5.59E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6273	4.19E-02	0.5541	0.048	5.60E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6405	4.17E-02	0.5550	0.048	5.60E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6537	4.16E-02	0.5559	0.049	5.61E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6668	4.15E-02	0.5569	0.049	5.62E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6800	4.13E-02	0.5578	0.049	5.62E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.6932	4.12E-02	0.5588	0.049	5.63E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7064	4.11E-02	0.5597	0.049	5.64E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7195	4.10E-02	0.5607	0.049	5.65E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7327	4.08E-02	0.5616	0.049	5.65E-06	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7457	3.36E-02	0.5654	0.112	1.27E-05	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7589	3.29E-02	0.5748	0.114	1.28E-05	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7721	3.23E-02	0.5847	0.116	1.29E-05	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7852	3.17E-02	0.5942	0.118	1.30E-05	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000
2.7984	3.11E-02	0.6036	0.119	1.31E-05	0.00E+00	1.96E-04	0	0.215	0.028	0.142	0.523	0.093	0.000

Table 3–8.   Perchloroethene output data, source synoptic inputs.

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{0L} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment ID	1	2	Air
0.0000	3.90E-02	0.3542	0.215	2.42E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0132	3.83E-02	0.3593	0.218	2.43E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0265	3.75E-02	0.3643	0.221	2.45E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0397	3.68E-02	0.3694	0.224	2.47E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0529	3.62E-02	0.3745	0.227	2.48E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0662	3.55E-02	0.3796	0.230	2.50E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0794	3.49E-02	0.3847	0.233	2.52E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.0926	3.43E-02	0.3897	0.236	2.53E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1062	3.40E-02	0.3914	0.101	1.25E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1197	3.38E-02	0.3924	0.101	1.25E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1332	3.36E-02	0.3934	0.102	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1467	3.34E-02	0.3944	0.102	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1602	3.32E-02	0.3955	0.102	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1737	3.31E-02	0.3965	0.103	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.1872	3.29E-02	0.3975	0.103	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2007	3.27E-02	0.3986	0.103	1.26E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2142	3.25E-02	0.3995	0.103	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2276	3.23E-02	0.4006	0.104	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2411	3.21E-02	0.4016	0.104	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2546	3.20E-02	0.4026	0.104	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2681	3.18E-02	0.4037	0.104	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2816	3.16E-02	0.4047	0.105	1.27E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.2951	3.14E-02	0.4057	0.105	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3086	3.13E-02	0.4067	0.105	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3221	3.11E-02	0.4078	0.105	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3356	3.09E-02	0.4087	0.106	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3490	3.08E-02	0.4098	0.106	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3625	3.06E-02	0.4108	0.106	1.28E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3760	3.04E-02	0.4118	0.106	1.29E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.3895	3.03E-02	0.4129	0.107	1.29E-05	0.00E+00	8.11E-04	0	1.000	0.000	0.000
0.4025	3.34E-02	0.4136	0.084	1.04E-05	4.09E-11	8.11E-04	2	0.901	0.099	0.000
0.4158	4.98E-02	0.4213	0.070	8.72E-06	1.11E-09	8.11E-04	2	0.592	0.408	0.000
0.4290	6.53E-02	0.4303	0.072	8.81E-06	1.11E-09	8.11E-04	2	0.441	0.559	0.000
0.4422	8.01E-02	0.4393	0.073	8.90E-06	1.11E-09	8.11E-04	2	0.352	0.648	0.000
0.4554	9.42E-02	0.4484	0.075	9.00E-06	1.11E-09	8.11E-04	2	0.292	0.708	0.000
0.4686	1.08E-01	0.4575	0.076	9.09E-06	1.11E-09	8.11E-04	2	0.250	0.750	0.000
0.4818	1.21E-01	0.4665	0.078	9.17E-06	1.11E-09	8.11E-04	2	0.218	0.782	0.000
0.4950	1.33E-01	0.4757	0.079	9.26E-06	1.11E-09	8.11E-04	2	0.194	0.806	0.000
0.5082	1.45E-01	0.4847	0.081	9.35E-06	1.11E-09	8.11E-04	2	0.174	0.826	0.000
0.5214	1.57E-01	0.4937	0.082	9.44E-06	1.11E-09	8.11E-04	2	0.158	0.842	0.000
0.5346	1.68E-01	0.5026	0.084	9.52E-06	1.11E-09	8.11E-04	2	0.145	0.855	0.000
0.5477	1.72E-01	0.5050	0.065	1.26E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.5614	1.70E-01	0.5007	0.065	1.25E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.5750	1.69E-01	0.4960	0.064	1.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.5887	1.68E-01	0.4918	0.064	1.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6024	1.66E-01	0.4875	0.063	1.23E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000

Table 3–8. Perchloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
0.6160	1.65E-01	0.4833	0.062	1.23E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6297	1.64E-01	0.4790	0.062	1.22E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6433	1.62E-01	0.4743	0.061	1.22E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6570	1.61E-01	0.4702	0.061	1.21E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6707	1.60E-01	0.4659	0.060	1.21E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6843	1.59E-01	0.4615	0.060	1.20E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.6980	1.57E-01	0.4572	0.059	1.20E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7116	1.56E-01	0.4529	0.058	1.19E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7253	1.55E-01	0.4485	0.058	1.18E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7390	1.53E-01	0.4442	0.057	1.18E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7526	1.52E-01	0.4399	0.057	1.17E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7663	1.51E-01	0.4356	0.056	1.17E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7799	1.50E-01	0.4312	0.056	1.16E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.7936	1.48E-01	0.4269	0.055	1.16E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8073	1.47E-01	0.4225	0.055	1.15E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8209	1.46E-01	0.4182	0.054	1.14E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8346	1.45E-01	0.4139	0.053	1.14E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8482	1.44E-01	0.4096	0.053	1.13E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8619	1.42E-01	0.4052	0.052	1.13E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8756	1.41E-01	0.4009	0.052	1.12E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.8892	1.40E-01	0.3966	0.051	1.11E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9029	1.39E-01	0.3922	0.051	1.11E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9165	1.37E-01	0.3879	0.050	1.10E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9302	1.36E-01	0.3836	0.050	1.26E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9438	1.35E-01	0.3793	0.049	1.25E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9575	1.33E-01	0.3749	0.048	1.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9712	1.32E-01	0.3706	0.048	1.23E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9848	1.31E-01	0.3662	0.047	1.22E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
0.9985	1.29E-01	0.3619	0.047	1.21E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0121	1.28E-01	0.3576	0.046	1.20E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0258	1.27E-01	0.3532	0.046	1.19E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0395	1.25E-01	0.3489	0.045	1.18E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0531	1.24E-01	0.3446	0.045	1.17E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0668	1.23E-01	0.3403	0.044	1.16E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0804	1.21E-01	0.3359	0.043	1.15E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.0934	1.20E-01	0.3333	0.047	8.55E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1066	1.16E-01	0.3448	0.063	9.03E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1197	1.11E-01	0.3576	0.066	9.20E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1328	1.07E-01	0.3704	0.068	9.36E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1459	1.03E-01	0.3833	0.070	9.52E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1589	1.02E-01	0.3839	0.067	8.34E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1721	1.02E-01	0.3734	0.065	8.22E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1853	1.02E-01	0.3630	0.063	8.11E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.1984	1.02E-01	0.3526	0.061	7.99E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2116	1.01E-01	0.3421	0.059	7.87E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2247	1.01E-01	0.3317	0.058	7.75E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2377	1.01E-01	0.3273	0.246	2.33E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000

Table 3–8. Perchloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
1.2512	1.00E-01	0.3265	0.245	2.33E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2647	1.00E-01	0.3256	0.245	2.32E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2782	9.97E-02	0.3247	0.244	2.32E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.2916	9.94E-02	0.3239	0.243	2.32E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3051	9.90E-02	0.3230	0.243	2.31E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3186	9.87E-02	0.3221	0.242	2.31E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3320	9.84E-02	0.3213	0.241	2.31E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3455	9.80E-02	0.3204	0.241	2.30E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3590	9.77E-02	0.3196	0.240	2.30E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3724	9.73E-02	0.3187	0.239	2.30E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3859	9.70E-02	0.3179	0.239	2.29E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.3994	9.67E-02	0.3170	0.238	2.29E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4128	9.63E-02	0.3162	0.237	2.29E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4263	9.60E-02	0.3153	0.237	2.29E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4398	9.57E-02	0.3144	0.236	2.28E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4533	9.53E-02	0.3136	0.235	2.28E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4667	9.50E-02	0.3127	0.235	2.28E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4802	9.47E-02	0.3118	0.234	2.27E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.4937	9.43E-02	0.3110	0.234	2.27E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5071	9.40E-02	0.3101	0.233	2.27E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5206	9.37E-02	0.3093	0.232	2.26E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5341	9.33E-02	0.3084	0.232	2.26E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5475	9.30E-02	0.3075	0.231	2.26E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5610	9.27E-02	0.3067	0.230	2.25E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5745	9.24E-02	0.3058	0.230	2.25E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.5879	9.20E-02	0.3049	0.229	2.25E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6014	9.17E-02	0.3041	0.228	2.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6149	9.14E-02	0.3032	0.228	2.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6284	9.11E-02	0.3024	0.227	2.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6418	9.07E-02	0.3015	0.226	2.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6551	5.36E-02	0.5036	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6686	5.23E-02	0.5045	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6821	5.10E-02	0.5050	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.6956	4.98E-02	0.5059	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7091	4.85E-02	0.5069	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7226	4.73E-02	0.5078	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7361	4.62E-02	0.5088	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7496	4.51E-02	0.5092	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7631	4.40E-02	0.5102	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7766	4.29E-02	0.5111	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.7902	4.19E-02	0.5121	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8037	4.08E-02	0.5130	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8172	3.99E-02	0.5139	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8307	3.89E-02	0.5144	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8442	3.80E-02	0.5154	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8577	3.70E-02	0.5163	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8712	3.62E-02	0.5172	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000

Table 3–8. Perchloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
1.8847	3.53E-02	0.5182	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.8977	3.45E-02	0.5187	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9112	3.43E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9247	3.42E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9382	3.42E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9517	3.41E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9652	3.40E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9788	3.39E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
1.9923	3.39E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0058	3.38E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0193	3.37E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0328	3.36E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0463	3.36E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0598	3.35E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0733	3.34E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.0868	3.33E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1003	3.33E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1138	3.32E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1274	3.31E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1409	3.30E-02	0.5187	0.026	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1541	3.28E-02	0.5191	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1672	3.21E-02	0.5201	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1803	3.14E-02	0.5210	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.1933	3.07E-02	0.5224	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2064	3.01E-02	0.5234	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2195	2.94E-02	0.5243	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2326	2.88E-02	0.5257	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2456	2.82E-02	0.5267	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2587	2.76E-02	0.5276	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2718	2.70E-02	0.5290	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2849	2.65E-02	0.5300	0.003	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.2979	1.78E-02	0.5305	0.039	8.83E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3112	1.78E-02	0.5314	0.046	5.12E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3243	1.77E-02	0.5324	0.047	5.12E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3375	1.77E-02	0.5333	0.047	5.13E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3507	1.76E-02	0.5342	0.047	5.14E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3639	1.75E-02	0.5352	0.047	5.14E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3770	1.75E-02	0.5361	0.047	5.15E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.3902	1.74E-02	0.5371	0.047	5.16E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4034	1.74E-02	0.5380	0.047	5.16E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4166	1.73E-02	0.5390	0.047	5.17E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4297	1.73E-02	0.5399	0.047	5.18E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4429	1.72E-02	0.5408	0.047	5.18E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4561	1.72E-02	0.5418	0.047	5.19E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4692	1.71E-02	0.5427	0.047	5.20E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4824	1.71E-02	0.5437	0.047	5.20E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.4956	1.70E-02	0.5446	0.048	5.21E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000

Table 3–8.   Perchloroethene output data, source synoptic inputs.—Continued

x (km)	c_i (µg/L)	Q (m³/s)	V (m/s)	k_{OL} (m/s)	$m_{i,in}$ (µg)	c_s (µg/L)	Source Apportionment			
							ID	1	2	Air
2.5088	1.70E-02	0.5456	0.048	5.21E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5219	1.69E-02	0.5465	0.048	5.22E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5351	1.69E-02	0.5475	0.048	5.23E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5483	1.68E-02	0.5484	0.048	5.23E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5615	1.68E-02	0.5493	0.048	5.24E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5746	1.67E-02	0.5503	0.048	5.25E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.5878	1.67E-02	0.5512	0.048	5.25E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6010	1.66E-02	0.5522	0.048	5.26E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6142	1.66E-02	0.5531	0.048	5.27E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6273	1.65E-02	0.5541	0.048	5.27E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6405	1.65E-02	0.5550	0.048	5.28E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6537	1.64E-02	0.5559	0.049	5.29E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6668	1.64E-02	0.5569	0.049	5.29E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6800	1.63E-02	0.5578	0.049	5.30E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.6932	1.63E-02	0.5588	0.049	5.31E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7064	1.62E-02	0.5597	0.049	5.31E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7195	1.62E-02	0.5607	0.049	5.32E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7327	1.61E-02	0.5616	0.049	5.33E-06	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7457	1.35E-02	0.5654	0.112	1.20E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7589	1.33E-02	0.5748	0.114	1.21E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7721	1.30E-02	0.5847	0.116	1.22E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7852	1.28E-02	0.5942	0.118	1.23E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000
2.7984	1.26E-02	0.6036	0.119	1.24E-05	0.00E+00	8.11E-04	0	0.140	0.860	0.000

Appendix 4. Example Physical/Chemical Properties for Selected Volatile Organic Compounds

[g/mol, grams per mole; mol/atm-m^3, moles per atmosphere-cubic meters; cm^3/mol, cubic centimeters per mole]

Compound	Molecular weight (g/mole)	Henry's Law Constant Parameterization (atm-m^3/mol)	Molar volume (cm^3/mol)
Acetone	58.08	[1]Exp(7.034+5043/T)	73.4
Benzene	78.12	[2]Exp(7.924+3918/T)	94.3
Methyl *tert*-butyl ether	88.15	[3]Exp(18.4+7666/T)	129.4
Chloroform	119.4	[4]Exp(9.824-4608/T)	84.9
1,1-Dichloroethane	98.96	[4]Exp(8.644-4131/T)	88.8
cis-1,2-Dichloroethene	96.94	[4]Exp(8.484-4196/T)	78.1
Trichloroethene	131.3	[5]Exp(7.854-3702/T)	94.3
Perchloroethene	165.8	[5]Exp(12.48-4931/T)	115.3

[1]Zhou and Mopper (1990).

[2]Leighton and Calo (1981).

[3]Robbins and others (1993).

[4]Gossett (1987).

[5]Ashworth and others (1988).

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