# Appendix A. SEAM3D Input

## A.1 General Information

Since SEAM3D is based on MT3D (Zheng, 1990), much of the input is identical for the two models, and a basic understanding of MT3D is the first step toward mastering SEAM3D. Users who are unfamiliar with MT3D will benefit from reading the MT3D technical documentation (Zheng, 1990). The following sections paraphrase and condense information from the MT3D technical documentation, while information relevant to the additional subroutines in SEAM3D is provided in greater detail. SEAM3D will not require detailed input or reserve computer memory for model options that are not specified by the user. For example, if dissolution of contaminants from a non-aqueous phase liquid (NAPL) is not simulated, then the user does not create the NAPL dissolution input file (see Section 4.2.6).

Estimation of model parameters for biodegradation may be based on laboratory measurements, published values, and theoretical estimates. To produce maximum flexibility, SEAM3D allows parameters to vary across the aquifer layers and among the various substrates and electron acceptors for biodegradation. However, in the absence of detailed information, the user is advised to enter identical parameter values to describe the layers and certain biodegradation processes. Thus, parameter estimation can be simplified when available data do not support a more detailed analysis. Further information on parameter estimation is included in the detailed input instructions (Sections 4.2.1 to 4.2.6).

### *A.1.1 Types of Input*

Like MT3D, input for SEAM3D may be formatted, list-directed, or unformatted.

**Formatted**

Input variables may be formatted as integer, real, character, or logical. In the detailed input instructions (Sections 4.2.1 to 4.2.6), the format column uses I to specify an integer, F for a real number, A for a character variable, and L for a logical variable. Input conventions follow the standards of the FORTRAN 77 language.

**List Directed**

List directed, or free format, input involves a sequence of values separated by blanks or commas. The list directed record terminates when a slash (/) is encountered, repeat counters are permitted, and each new record should begin on a new line of the input file.

**Unformatted**

Unformatted files contain binary characters and must be written and read by the computer. Relative to formatted files, unformatted files are smaller and can be processed more readily.

### *A.1.2 Array Readers*

Most of the input data for SEAM3D is handled by the subroutines IARRAY and RARRAY in the utility module of the program. IARRAY reads one or two dimensional integer arrays, and RARRAY reads one or two dimensional real arrays. Three dimensional arrays are handled by reading a two dimensional areal array for each model layer. Each time an array reader is called, it initially reads an array control record, which occupies a single line of the input filed and is formatted as follows:

| Record: | IREAD | CNSTNT (real) or ICONST (integer) | FMTIN | IPRN |
|---|---|---|---|---|
| Format: | I10 | F10.0 (real) or I10 (integer) | A20 | I10 |

If IREAD = 0, then RARRAY sets all elements of the array equal to CNSTNT, or IARRAY sets all elements equal to ICONST.

If IREAD = 100, then array values (entered on the lines following the array control record) are read in the format specified by FMTIN.

If IREAD = 101, then array values are read as blocks, which are entered on the lines following the array control record. The first line contains only the record NBLOCK, which is an integer specifying the number of blocks to follow. Each block occupies a single line, consisting of I1, I2, J1, J2, VALUE; where I1 is the index of the first row of the block, I2 is the index of the last row, J1 is the index of the first column of the block, J2 is the index of the last column, and VALUE is the value assigned to array elements within the block.

If IREAD = 102, then array values are read as zones.

If IREAD = 103, then array values are read in list directed format.

If IREAD is equal to a nonzero value other than 100, 101, 102, or 103, then array values are read from a separate file. If IREAD is positive, then IREAD is the unit number for the separate file, which is formatted according to FMTIN. If IREAD is negative, then the separate file is unformatted, and the absolute value of IREAD is its unit number.

If IREAD ≠ 0 and CNSTNT or ICONST ≠ 0, then all elements in the array are multiplied by CNSTNT or ICONST.

The format specifier FMTIN must be enclosed in parentheses.

If IREAD ≠ 0, then IPRN acts as a flag to indicate whether the array will be printed for checking. The array will not be printed in IPRN is negative.

### *A.1.3 Units*

Like MT3D, SEAM3D requires the user to specify units and use consistent units for all input and output variables. In addition, the time unit must be consistent with that used in the flow model. The single exception to this rule involves the concentrations of solid phase electron acceptors, which are entered as mass of electron acceptor per 1 x $10^6$ mass of soil solids (e.g. micrograms per gram). Units of METERS for length and GRAMS for mass are convenient because they produce concentration units of grams per cubic meter, which is equivalent to milligrams per liter.

## A.2 Input Instructions

Many of the input lines are identical in both SEAM3D and MT3D. In the following sections, these lines will be given the same numbering style as in the MT3D user guide (e.g., A1 for the first line of the Basic Transport File). If SEAM3D alters an MT3D input line, then the number is followed by an asterisk (e.g., A3* for the third line of the Basic Transport File). If SEAM3D uses an input line that is not included in MT3D, then the line number is given an "S" to indicate that it is unique to SEAM3D (e.g., AS1 for the fourth line of the Basic Transport File). Many input lines in SEAM3D are required only if certain model options are switched on. For example, if no inorganic nutrients are simulated, then nutrient parameters such as initial concentrations are not entered. In the detailed input instructions, certain input lines are grouped

in boxes underneath the conditional statement that indicates whether the lines should be included in the file. Often these groups are preceded by a line of descriptive text that helps the user locate the lines in the file for editing. In order to illustrate input structure, example input files are included with the SEAM3D source code and executable files. It is highly recommended that the user prepare input files by modifying existing files

The terms “outer loop” and “inner loop” are used throughout the detailed input instructions to indicate the order for entering lines describing arrays of more than two dimensions. For example, in line AS6 of the Basic Transport Package, the subroutine IARRAY must be called repeatedly to read the four dimensional array IAEBND(ncol, nrow, nlay, nelec). Each time IARRAY is called, it reads a two dimensional array IAEBND(ncol, nrow) for specified values of nlay and nelec. Thus the model must loop through values for nlay and nelec, going through the inner loop first. In other words, for the first electron acceptor, (nelec = 1), IARRAY is called for each model layer before moving to the second electron acceptor (nelec = 2).

### *A.2.1 Input Instructions for the Basic Transport Package*

This input file contains information describing the model configuration, initial conditions, and output options. It must be created for all simulations and is read on unit 1.

Initial concentrations of hydrocarbon substrates, electron acceptors, inorganic nutrients, products, and nonbiodegradable tracers should be based on concentrations measured in the field. If a certain process is not included in the simulation, then the corresponding parameters are not entered and need not be estimated. For example, if nitrate reduction is not simulated, then initial and minimum concentrations of nitrate are not entered in the basic transport package. The minimum concentrations of substrates, electron acceptors, and nutrients may be set to zero unless measured data indicate otherwise.

Due to the difficulty in quantifying aquifer microbes, data on the initial microbial biomass ($M_x$) may not be available, and only a rough estimate of $M_x$ may be obtained. Under pristine conditions, when the groundwater contains significant $O_2$, it can be assumed that aerobic biomass predominates. Anaerobic microbes would exist only in anaerobic microsites that develop within soil aggregates. Thus, the value of $M_x$ for each anaerobic biomass can be estimated as an order of magnitude lower than the aerobic biomass. In general, if $M_x$ for the anaerobes is on the order of 0.01 g $m^{-3}$, then the anaerobic biomass must undergo significant growth before the population exerts a significant impact on biodegradation. For the aerobes, $M_x$ equal to 0.3 g $m^{-3}$ corresponds to 1 x $10^6$ cells $cm^{-3}$, assuming a cell volume of 1 $\mu m^3$, cell density of 1.0 g $cm^{-3}$, and aquifer porosity of 0.3. This number of cells usually allows significant aerobic utilization of substrates to occur without additional microbial growth.

For the Observation Point output files, (see input line A19*), SEAM3D prints out the vertically averaged concentrations at the specified areal location as well as the actual concentrations in the block. If the user specifies a *k* index for upper and lower layers, then the vertical average will include only these layers and the layers in between. For example, if KINIO = 1 and KFINO = 3, then the vertical average will include only layers 1, 2 and 3. If KINIO and KFINO are set to zero or left blank, then the vertical average is computed over all model layers.

This averaging process also applies to the Transect output files (line AS37) and the Surfer output files (line AS39).

| Line | Variable | Format | Description |
|---|---|---|---|
| A1 | HEADNG(1) | A80 | Title |
| A2 | HEADNG(2) | A80 | Title |
| A3* | NLAY | I10 | Total number of layers |
| | NROW | I10 | Total number of rows |
| | NCOL | I10 | Total number of columns |
| | NPER | I10 | Total number of stress periods |
| | IBIO | I10 | Flag for biodegradation<br>= 0 no biodegradation (same as MT3D)<br>= 1 biodegradation simulated |
| ***(Enter line AS1 if IBIO = 1)*** | | | |
| AS1 | NHCAR | I10 | Total number of biodegradable substrates<br>$1 \leq NHCAR \leq 8$ |
| | NNUTR | I10 | Total number of inorganic nutrients<br>$0 \leq NNUTR \leq 5$ |
| | NTRAC | I10 | Total number of non-biodegradable tracers<br>$0 \leq NTRAC \leq 5$ |
| | NDAUT | I10 | Total number of daughter products<br>$0 \leq NDAUT \leq NHCAR$ |
| | IDISS | I10 | Flag for NAPL dissolution<br>= 0 no NAPL dissolution<br>= 1 NAPL dissolution |
| A4 | TUNIT | A4 | Name for time unit |
| | LUNIT | A4 | Name for length unit |
| | MUNIT | A4 | Name for mass unit |
| A5 | TRNOPT(4) | 4L2 | Flags for major transport options: advection, dispersion, source/sink mixing, and chemical reactions. Enter T to include the option in the simulation; enter F to omit the option. |

***(Enter lines AS2 through AS4 if IBIO = 1)***

| | | | |
|---|---|---|---|
| AS2 | STOCHOPT | L2 | Flag for spatial variability option for maximum specific rate of substrate utilization. Enter T to allow the parameter to vary in space; enter F for constant value. |
| AS3 | CLNOPT(6) | 6L2 | Flags for microcolony options: aerobes, NO3 reducers, Mn(IV) reducers, Fe(III) reducers, SO4 reducers, methanogens. Enter T to include the microcolony in the simulation; enter F to omit. |
| AS4 | ENDOPT(4) | 4L2 | Flags for product options: NO2, Mn(II), Fe(II), H2S. Enter T to include the product in the simulation; enter F to omit. Note that ENDOPT(5) for CH4 is automatically set from CLNOPT(6) for methanogens. |
| A6 | LAYCON(nlay) | 40I2 | Code for layer type<br>= 0 Confined<br>≠ 0 unconfined or convertible<br>(use as many lines as necessary) |
| A7 | DELR(ncol) | RARRAY | Block width along rows (Δx) |
| A8 | DELC(nrow) | RARRAY | Block width along columns (Δy) |
| A9 | HTOP(ncol, nrow) | RARRAY | Top elevation of blocks in layer 1<br>(same datum as heads in flow model) |
| A10 | DZ(ncol, nrow, nlay) | RARRAY | Block thickness:<br>Enter DZ(ncol, nrow) for each layer |
| A11 | PRSITY(ncol, nrow, nlay) | RARRAY | Effective porosity:<br>Enter PRSITY(ncol, nrow) for each layer |

***(Enter line A12* if IBIO = 0)***

| | | | |
|---|---|---|---|
| A12* | IATBND(ncol, nrow, nlay, ntrac) | IARRAY | Boundary indicator array:<br>Enter IATBND(ncol, nrow) for each layer; NTRAC must equal 1<br>= 0 Inactive concentration block<br>> 0 Variable concentration block<br>< 0 Constant concentration block |

***(Enter lines AS5 through AS16 if IBIO = 1)***

| | | | |
|---|---|---|---|
| AS5 | Descriptive text | None | "Electron Acceptor Boundary Arrays" |
| AS6 | IAEBND(ncol, nrow, nlay, nelec) | IARRAY | Boundary indicator array:<br>Enter IAEBND(ncol, nrow) for each layer (inner loop) and for each aqueous phase electron acceptor (outer loop)<br>NELEC is the total number of aqueous phase electron acceptors<br>(calculated automatically from the microcolony options) |
| AS7 | Descriptive text | None | "Hydrocarbon Boundary Arrays" |
| AS8 | IAHBND(ncol, nrow, nlay, nhcar) | IARRAY | Boundary indicator array:<br>Enter IAHBND(ncol, nrow) for each layer (inner loop) and for each hydrocarbon (outer loop) |
| AS9 | Descriptive text | None | "Nutrient Boundary Arrays" |
| AS10 | IANBND(ncol, nrow, nlay, nnutr) | IARRAY | Boundary indicator array:<br>Enter IANBND(ncol, nrow) for each layer (inner loop) and for each inorganic nutrient (outer loop) |
| AS11 | Descriptive text | None | "Product Boundary Arrays" |
| AS12 | IAPBND(ncol, nrow, nlay, nprod) | IARRAY | Boundary indicator array:<br>Enter IAPBND(ncol, nrow) for each layer (inner loop) and for each product (outer loop)<br>NPROD is the total number of products, including CH4 |
| AS13 | Descriptive text | None | "Daughter Boundary Arrays" |
| AS14 | IADBND(ncol, nrow, nlay, ndaut) | IARRAY | Boundary indicator array:<br>Enter IADBND(ncol, nrow) for each layer (inner loop) and for each daughter (outer loop) |
| AS15 | Descriptive text | None | "Tracer Boundary Arrays" |
| AS16 | IATBND(ncol, nrow, nlay, ntrac) | IARRAY | Boundary indicator array:<br>Enter IATBND(ncol, nrow) for each layer (inner loop) and for each tracer (outer loop) |

***(Enter line A13* if IBIO = 0)***

| | | | |
|---|---|---|---|
| A13* | ATOLD(ncol, nrow, nlay, ntrac) | RARRAY | Starting concentration:<br>Enter ATOLD(ncol, nrow) for each layer; NTRAC must equal 1 |

***(Enter lines AS17 through AS34 if IBIO = 1)***

| | | | |
|---|---|---|---|
| AS17 | Descriptive text | None | "Electron Acceptor Starting Concentrations" |
| AS18 | AEOLD(ncol, nrow, nlay, nelec)<br>or<br>SEOLD(ncol, nrow, nlay, nslid) | RARRAY | Starting concentrations:<br>Enter AEOLD(ncol, nrow) or SEOLD(ncol, nrow) for each layer (inner loop) and for each electron acceptor (outer loop). Electron acceptors are read in the following order: $O_2$, $NO_3$, Fe(III), Mn(IV), $SO_4$. NSLID is the total number of solid phase electron acceptors (calculated automatically from the microcolony options) |
| AS19 | AEMIN(nelec) or SEMIN(nslid) | F10.0 | Minimum concentrations:<br>Enter AEMIN or SEMIN after AEOLD(ncol, nrow) or SEOLD(ncol, nrow) for each electron acceptor |
| AS20 | Descriptive text | None | "Hydrocarbon Starting Concentrations" |
| AS21 | AHOLD(ncol, nrow, nlay, nhcar) | RARRAY | Starting concentrations:<br>Enter AHOLD(ncol, nrow) for each layer (inner loop) and for each hydrocarbon (outer loop) |
| AS22 | AHMIN(nhcar) | F10.0 | Minimum concentrations:<br>Enter AHMIN after AHOLD(ncol, nrow) for each hydrocarbon |
| AS23 | Descriptive text | None | "Nutrient Starting Concentrations" |
| AS24 | ANOLD(ncol, nrow, nlay, nnutr) | RARRAY | Starting concentrations:<br>Enter ANOLD(ncol, nrow) for each layer (inner loop) and for each inorganic nutrient (outer loop) |
| AS25 | ANMIN(nnutr) | F10.0 | Minimum concentrations:<br>Enter ANMIN after ANOLD(ncol, nrow) for each nutrient |
| AS26 | Descriptive text | None | "Product Starting Concentrations" |
| AS27 | APOLD(ncol, nrow, nlay, nprod) | RARRAY | Starting concentrations:<br>Enter APOLD(ncol, nrow) for each layer (inner loop) and for each product (outer loop) |
| AS28 | Descriptive text | None | "Daughter Starting Concentrations" |
| AS29 | ADOLD(ncol, nrow, nlay, ndaut) | RARRAY | Starting concentrations:<br>Enter ADOLD(ncol, nrow) for each layer (inner loop) and for each daughter |

| | | | |
|---|---|---|---|
| | | | (outer loop) |
| AS30 | Descriptive text | None | "Microcolony Starting Concentrations" |
| AS31 | XMOLD(ncol, nrow, nlay, nclny) | RARRAY | Starting concentrations:<br>Enter XMOLD(ncol, nrow) for each layer (inner loop) and for each microcolony (outer loop).<br>NCLNY is the total number of microcolonies in the simulation |
| AS32 | XMMIN | RARRAY | Minimum conc. for all microcolonies:<br>Enter XMMIN after the last entry of XMOLD(ncol, nrow) |
| AS33 | Descriptive text | None | "Tracer Starting Concentrations" |
| AS34 | ATOLD(ncol, nrow, nlay, ntrac) | RARRAY | Starting concentrations:<br>Enter ATOLD(ncol, nrow) for each layer (inner loop) and for each tracer (outer loop) |
| A14 | CINACT | F10.0 | Value indicating inactive block |
| A15 | IFMTCN | I10 | Print format code for concentrations<br>> 0 wrap form<br>< 0 strip form<br>= 0 not printed |
| | IFMTNP | I10 | Print format code for particles<br>(same convention as IFMTCN) |
| | IFMTRF | I10 | Print format code for retardation factor (same convention as IFMTCN) |
| | IFMTDP | I10 | Print format code for dispersion coefficient<br>(same convention as IFMTCN) |
| | SAVUCN | L10 | Flag for saving concentrations in unformatted files for continuation run or post processing<br>(SAVUCN = T to save concentrations) |
| A16 | NPRS | I10 | Flag for frequency of model output<br>> 0 output times specified by TIMPRS(NPRS)<br>< 0 output saved when transport step number is a multiple of NPRS<br>= 0 output saved only at the end of the simulation |
| ***(Enter line A17 only if NPRS > 0)*** | | | |
| A17 | TIMPRS(NPRS) | 8F10.0 | Time at which concentrations are printed to the main output and unformatted files<br>(Enter as many lines as necessary) |

| | | | |
|---|---|---|---|
| A18* | NOBS | I10 | Number of observation points |
| | NPRTO | I10 | Frequency for writing observations<br>NPRTO ≤ 1 write for all transport steps<br>NPRTO > 1 write every NPRTO transport steps |

***(Enter line A19* NOBS times if NOBS > 0)***

| | | | |
|---|---|---|---|
| A19* | KOBS, IOBS, JOBS | 3I10 | Layer, row, and column indices of the observation points (concentrations will be saved at each transport step) |
| | KINIO, KFINO | 2I10 | *k* indices of the upper and lower layers for computing vertically averaged concentrations |

***(Enter lines AS35 through AS39 if IBIO = 1)***

| | | | |
|---|---|---|---|
| AS35 | KSCR, ISCR,JSCR | 3I10 | Layer, row, and column indices for screen output |
| AS36 | NTSECT | I10 | Number of times for output of transect information |
| | IDIR | I10 | Transect direction<br>= 1 transect runs along the x-direction<br>= 2 transect runs along the y-direction |
| | INODD | I10 | *i* or *j* index for the transect location |
| AS37 | TRTIME(NTSECT) | F10.0 | Time when concentrations are printed to transect files |
| | KINIT(NTSECT) | I10 | *k* index of the upper layer for computing vertically averaged concentrations |
| | KFINT(NTSECT) | I10 | *k* index of the lower layer for computing vertically averaged concentrations<br>Enter NTSECT lines |
| AS38 | NTSURF | I10 | Number of times for output of SURFER data files |
| AS39 | SUTIME(NTSURF) | F10.0 | Time when concentrations are printed to SURFER data files |
| | KINIS(NTSURF) | I10 | *k* index of the upper layer for computing vertically averaged concentrations |
| | KFINS(NTSURF) | I10 | *k* index of the lower layer for computing vertically averaged concentrations<br>Enter NTSURF lines |
| A20* | CHKMAS | L10 | Flag for saving mass balance information (CHKMAS = T to save information) |
| | NPRTM | I10 | Frequency for writing mass information |

NPRTM ≤ 1 write for all transport steps
NPRTM > 1 write every NPRTM transport steps

***(Repeat lines A21 through A23 for each stress period***

| | | | |
|---|---|---|---|
| A21 | PERLEN | F10.0 | Time length of the current stress period |
| | NSTP | I10 | Number of time steps in the current stress period |
| | TSMULT | F10.0 | Time step multiplier<br>> 0 length of each time step is calculated from a geometric progression<br>≤ 0 length of each time step is read from TSMULT(NSTP) |

***(Enter line A22 only if TSMULT ≤ 0)***

| | | | |
|---|---|---|---|
| A22 | TSLNGH(NSTP) | 8F10.0 | Length of each time step<br>Enter as many lines as necessary |
| A23 | DTO | F10.0 | Transport step size<br>> 0 DTO is used, unless the calculated transport step size is smaller<br>≤ 0 Calculated transport step size is used |
| | MXSTRN | I10 | Maximum number of transport steps allowed for one time step of the head solution |

### *A.2.2 Input Instructions for the Advection Package*

This input file must be created only if the Advection Package is specified in the Basic Transport Package; i.e., TRNOPT(1) is set to "T". Input for advection is read on unit 2, and advection is normally included in all simulations. Because SEAM3D only supports the finite difference solution for advection, parameters for particle tracking are not required.

| Line | Variable | Format | Description |
|---|---|---|---|
| B1 | MIXELM | I10 | Flag indicating advection solution method<br>Must set MIXELM = 0 for upstream finite difference method |
| | PERCEL | F10.0 | Courant number (generally, PERCEL ≤ 0.2) |
| | MXPART | I10 | Not used by SEAM3D, so any integer may be entered |

### *A.2.3 Input Instructions for the Dispersion Package*

This input file must be created only if the Dispersion Package is specified in the Basic Transport Package; i.e., TRNOPT(2) is set to "T". Input for dispersion is read on unit 3, and dispersion is normally included in all simulations. The Dispersion Package is identical for SEAM3D and MT3D.

| Line | Variable | Format | Description |
|---|---|---|---|
| C1 | AL(ncol, nrow, nlay) | RARRAY | Longitudinal dispersivity:<br>Enter AL(ncol, nrow) for each layer |
| C2 | TRPT(nlay) | RARRAY | Ratio of the horizontal transverse dispersivity to the longitudinal dispersivity:<br>Enter a value for each layer |
| C3 | TRPV(nlay) | RARRAY | Ratio of the vertical transverse dispersivity to the longitudinal dispersivity:<br>Enter a value for each layer |
| C4 | DMCOEF(nlay) | RARRAY | Effective molecular diffusion coefficient:<br>Enter a value for each layer |

### *A.2.4 Input Instructions for the Source/Sink Mixing Package*

This input file must be created if source/sink options (including constant head or general-head-dependent boundary conditions) are specified in the flow model. It is also necessary to specify the Source/Sink Mixing Package in the Basic Transport Package; i.e., TRNOPT(3) is set to T. Input for source/sink mixing is read on unit 4 The location and rates for the fluxes (due to wells, drains, recharge, evapotranspiration, rivers, and general- head-dependent boundary conditions) are obtained from the flow solution through the unformatted head and flow file. If a flux is positive, then it acts as a source, and concentrations must be specified. If a flux is negative, then it acts as a sink, and concentrations are set equal to the current concentrations within the block.

| Line | Variable | Format | Description |
|---|---|---|---|
| D1 | FWEL | L2 | Flag for the well option |
| | FDRN | L2 | Flag for the drain option |
| | FRCH | L2 | Flag for the recharge option |
| | FEVT | L2 | Flag for the evapotranspiration option |
| | FRIV | L2 | Flag for the river option |
| | FGHB | L2 | Flag for the general-head-dependent boundary option<br>Any of the above flags must be set to T if the corresponding option is used in the flow model; otherwise set to F |
| D2 | MXSS | I10 | Maximum number of point sources/sinks simulated in the flow model, including constant head blocks, wells, drains, rivers, and general-head-dependent boundary blocks. Recharge and evapotranspiration are not counted.<br>MXSS should be minimized to conserve computer memory. |

***(Repeat the following lines for each stress period***

***(Enter line D3 only if FRCH = T)***

| | | | |
|---|---|---|---|
| D3 | INCRCH | I10 | Flag for recharge flux in the current stress period<br>INCRCH ≥ 0 concentrations in recharge flux will be read as arrays<br>INCRCH < 0 concentrations in recharge flux will be used from the preceding stress period. If INCRCH < 0 for the first stress period, the model sets concentrations to zero by default |

***(Enter line D4* if IBIO = 0 and FRCH = T and INCRCH ≥ 0)***

| | | | |
|---|---|---|---|
| D4* | ATRCH(ncol, nrow, ntrac) | RARRAY | Concentration in recharge flux; NTRAC must equal 1 |

***(Enter lines DS1 through DS12 if IBIO = 1 and FRCH = T and INCRCH ≥ 0)***

| | | | |
|---|---|---|---|
| DS1 | Descriptive text | None | "Elec. Acceptor Concentration in Recharge" |
| DS2 | AERCH(ncol, nrow, nelec) | RARRAY | Concentrations in recharge flux:<br>Enter AERCH(ncol, nrow) for each aqueous phase electron acceptor |
| DS3 | Descriptive text | None | "Hydrocarbon Concentration in Recharge" |
| DS4 | AHRCH(ncol, nrow, nhcar) | RARRAY | Concentrations in recharge flux:<br>Enter AHRCH(ncol, nrow) for each hydrocarbon |
| DS5 | Descriptive text | None | "Nutrient concentration in Recharge" |
| DS6 | ANRCH(ncol, nrow, nnutr) | RARRAY | Concentrations in recharge flux:<br>Enter ANRCH(ncol, nrow) for each nutrient |
| DS7 | Descriptive text | None | "Product concentration in Recharge" |
| DS8 | APRCH(ncol, nrow, nprod) | RARRAY | Concentrations in recharge flux:<br>Enter APRCH(ncol, nrow) for each product |
| DS9 | Descriptive text | None | "Daughter concentration in Recharge" |
| DS10 | ADRCH(ncol, nrow, ndaut) | RARRAY | Concentrations in recharge flux:<br>Enter ADRCH(ncol, nrow) for each daughter |
| DS11 | Descriptive text | None | "Tracer concentration in Recharge" |
| DS12 | ATRCH(ncol, nrow, ntrac) | RARRAY | Concentrations in recharge flux:<br>Enter ATRCH(ncol, nrow) for each tracer |

***(Enter line D5 only if FEVT = T)***

| | | | |
|---|---|---|---|
| D5 | INCEVT | I10 | Flag for the evapotranspiration flux for the current stress period<br>INCEVT ≥ 0 concentrations in evapotranspiration flux will be read as arrays<br>INCEVT < 0 concentrations in evapotranspiration flux will be used from the preceding stress period. |

***(Enter line D6* if IBIO = 0 and FEVT = T and INCEVT ≥ 0)***

| | | | |
|---|---|---|---|
| D6* | ATEVT(ncol, nrow, ntrac) | RARRAY | Concentration in evapotranspiration flux; NTRAC must equal 1 |

***(Enter lines DS13 through DS24 if IBIO = 1 and FEVT = T and INCEVT ≥ 0)***

| | | | |
|---|---|---|---|
| DS13 | Descriptive text | None | "Elec. Acceptor Conc. in Evapotranspir." |
| DS14 | AEEVT(ncol, nrow, nelec) | RARRAY | Concentrations in evapotranspiration flux: Enter AEEVT(ncol, nrow) for each aqueous phase electron acceptor |
| DS15 | Descriptive text | None | "Hydrocarbon Conc. in Evapotranspiration" |
| DS16 | AHEVT(ncol, nrow, nhcar) | RARRAY | Concentrations in evapotranspiration flux: Enter AHEVT(ncol, nrow) for each hydrocarbon |
| DS17 | Descriptive text | None | "Nutrient conc. in Evapotranspiration" |
| DS18 | ANEVT(ncol, nrow, nnutr) | RARRAY | Concentrations in evapotranspiration flux: Enter ANEVT(ncol, nrow) for each nutrient |
| DS19 | Descriptive text | None | "Product conc. in Evapotranspiration" |
| DS20 | APEVT(ncol, nrow, nprod) | RARRAY | Concentrations in evapotranspiration flux: Enter APEVTH(ncol, nrow) for each product |
| DS21 | Descriptive text | None | "Daughter conc. in Evapotranspiration" |
| DS22 | ADEVT(ncol, nrow, ndaut) | RARRAY | Concentrations in evapotranspiration flux: Enter ADEVTH(ncol, nrow) for each daughter |
| DS23 | Descriptive text | None | "Tracer conc. in Evapotranspiration" |
| DS24 | ATEVT(ncol, nrow, ntrac) | RARRAY | Concentrations in evapotranspiration flux: Enter ATEVT(ncol, nrow) for each tracer |

| | | | |
|---|---|---|---|
| D7 | NSS | I10 | Number of point sources where concentrations must be specified. Unspecified concentrations at point sources will be set to zero. |

***(Enter line D8 only if NSS > 0)***

| | | | |
|---|---|---|---|
| D8 | KSS | I10 | Layer number of point source |
| | ISS | I10 | Row number of point source |
| | JSS | I10 | Column number of point source |
| | CSS | F10.0 | If ibio = 0, CSS is the specified conc. of the single contaminant (as in MT3D)<br>If ibio = 1, CSS is not used; any number may be specified |
| | ITYPE | I10 | Type of point source<br>ITYPE = 1 constant head<br>ITYPE = 2 well block<br>ITYPE = 1 drain<br>ITYPE = 1 river<br>ITYPE = 1 general-head-dependent boundary condition |

***(Enter lines DS25 through DS36 only if IBIO = 1)***

| | | | |
|---|---|---|---|
| DS25 | Descriptive text | None | "Electron Acceptor Point Source Conc." |
| DS26 | SSE | RARRAY | Point source concentrations:<br>Enter SSE for each aqueous phase electron acceptor |
| DS27 | Descriptive text | None | "Hydrocarbon Point Source Concentration" |
| DS28 | SSH | RARRAY | Point source concentrations: Enter SSH for each hydrocarbon |
| DS29 | Descriptive text | None | "Nutrient Point Source concentration" |
| DS30 | SSN | RARRAY | Point source concentrations:<br>Enter SSN for each nutrient |
| DS31 | Descriptive text | None | "Product Point Source concentration" |
| DS32 | SSP | RARRAY | Point source concentrations:<br>Enter SSP for each product |
| DS33 | Descriptive text | None | "Daughter Point Source concentration" |
| DS34 | SSD | RARRAY | Point source concentrations:<br>Enter SSD for each daughter |
| DS35 | Descriptive text | None | "Tracer Point Source Concentration" |
| DS36 | SST | RARRAY | Point source concentrations:<br>Enter SST for each tracer |

### *A.2.5 Input Instructions for the Reaction Package*

This input file must be created only if the Reaction Package is specified in the Basic Transport Package; i.e., TRNOPT(4) is set to "T". Input is read on unit 9, and it includes the biodegradation parameters.

In order to reflect the high rate and energy yield of aerobic metabolism, parameters controlling aerobic utilization, growth, and death should generally be much higher than those of the anaerobic processes. The maximum specific rate of substrate utilization ($\nu^{max}_{x,ls,le}$) may be based on laboratory or field estimates. Certain substrates, such as those in the alkane group, are resistant to anaerobic biodecay, so $\nu^{max}_{x,ls,le}$ for alkanes may be set to zero for each anaerobic process. Alkanes would still biodegrade using oxygen. For aerobic biodegradation of hydrocarbons, laboratory estimates of $\nu^{max}_{x,ls,le}$ have been reported as 1.0 $day^{-1}$ (Kindred and Celia, 1989), 1.7 $day^{-1}$ (Borden and Bedient, 1986), 3.5 to 8.0 $day^{-1}$ (Arcangeli and Arvin, 1992), and 8.3 to 9.9 $day^{-1}$ (Chen et al., 1992). Biodegradation rates in the field may be much lower than observed in the laboratory. A field study by MacIntyre et al. (1993) found that aerobic biodecay of benzene could be approximated by a pseudo-first order rate constant of 0.0070 $day^{-1}$. Chapelle and Lovley (1990) reported that microbial metabolic rates based on laboratory incubations may overpredict in situ rates by two orders of magnitude.

Values of the half saturation coefficients for substrates ($K^{s}_{x,ls,le}$) and electron acceptors ($K^{e}_{x,le}$) may be based on literature values if no measurements are available. For hydrocarbons, $K^{s}_{x,ls,le}$ has been reported in the range of 0.1 g $m^{-3}$ (Kindred and Celia, 1989), 0.13 g $m^{-3}$ (Borden and Bedient, 1986), 0.6 g $m^{-3}$ (Arcangeli and Arvin, 1992), 1.88 to 4.55 g $m^{-3}$ (Chang et al., 1993), 12.2 to 17.4 g $m^{-3}$ (Chen et al., 1992). For oxygen, $K^{e}_{x,le}$ has been reported as 0.10 g $m^{-3}$ (Borden and Bedient, 1986; Kindred and Celia, 1989; Chen et al., 1992). For nitrate, $K^{e}_{x,le}$ has been reported as 0.1 g $m^{-3}$ (Kindred and Celia, 1989), and 2.6 g $m^{-3}$ (Chen et al., 1992). With the exception of oxygen, values for half saturation coefficients are reported over a wide range, but

SEAM3D model results are generally much more sensitive to biomass concentration and $\nu^{max}_{x,ls,le}$ than to the half saturation coefficients.

The yield coefficient ($Y_{x,ls,le}$) for aerobes is often estimated as 0.5 g $g^{-1}$ (Arcangeli and Arvin, 1992; Borden and Bedient, 1986; Chen et al., 1992; Wodzinski and Johnson, 1968), although values as low as 0.25 have been used (Kindred and Celia, 1989). For anaerobes, $Y_{x,ls,le}$ is usually lower than for aerobes, with 0.2 g $g^{-1}$ being the theoretical maximum yield under sulfate reducing conditions (Edwards et al., 1992). It is recommended that the user allow SEAM3D to calculate values for the effective death terms ($k^{bk}_{d_x}$) internally, using the method described in Section 2.1.4.

When an inhibition coefficient ($\kappa_{le,li}$) is assigned a small value relative to its corresponding electron acceptor (EA), the EA must be essentially depleted before utilization of the next EA begins. In contrast, the inhibition process becomes insignificant if $\kappa_{le,li}$ is assigned a large value. Numerous values for inhibition coefficients have been reported. For inhibition by oxygen, $\kappa_{le,li}$ values vary between 0.01 and 0.1 g $m^{-3}$ (Kindred and Celia, 1989; Chen et al., 1992). Research has shown that methanogenesis may predominate over $SO_4^{2-}$ reduction when the $SO_4^{2-}$ concentration falls between 0.6 to 1.4 g $m^{-3}$ (Vroblesky et al., 1996). Thus the value of $\kappa_{le,li}$ for $SO_4^{2-}$ inhibition of methanogenesis should be within a similar range. In general, values of $\kappa_{le,li}$ for a particular inhibitor need not vary among the EA processes that are inhibited. For example, a value of $\kappa_{le,li}$ = 0.1 g $m^{-3}$ could be used to describe oxygen inhibition of all of the anaerobic processes. Values of $\kappa_{le,li}$ may be adjusted during calibration to match measured concentrations of products.

EA use coefficients ($\gamma_{x,ls,le}$) can be estimated from the stoichiometric relationship between each EA and the corresponding substrate. For aromatic hydrocarbons, there is little variation in the stoichiometry, and toluene may be used as a representative compound. Thus values for $\gamma_{x,ls,le}$ should be approximately equal to 3.1 g $g^{-1}$ for $O_2$, 4.8 g $g^{-1}$ for $NO_3^-$, 42.0 g $g^{-1}$ for Fe(III), 4.5 g $g^{-1}$ for $SO_4^{2-}$ (Borden et al., 1995), and 18.0 g $g^{-1}$ for Mn(IV) (Baedecker et al., 1993). The actual value of $\gamma_{x,ls,le}$ will depend somewhat on the specific hydrocarbon, and the amount of microbial assimilation of substrate into cell material. The generation term for methane ($\zeta_{x,ls}$) can

be estimated as 0.8 g $g^{-1}$, based on the stoichiometric relationship between toluene and methane (Borden et al., 1995). The EA generation terms ($\zeta_{x,le}$) can also be based on stoichiometric relationships. If $N_2$ is the final product of nitrate reduction, then $\zeta_{x,le}$ should be close to 0.5 g $g^{-1}$. For sulfide production, $\zeta_{x,le}$ should be close to 1.0 g $g^{-1}$ (Edwards et al., 1992). During calibration, the generation term for Fe(II) will often need to be reduced from its theoretical value to match the measured concentrations of Fe(II). This reduction is necessary because Fe(II) can react chemically with compounds such as $SO_4^{2-}$; thus, only a fraction of the Fe(II) produced by microbes may be measured in the groundwater (Lovley et al., 1994).

| Line | Variable | Format | Description |
|---|---|---|---|
| ***(Enter line E1 if IBIO = 0)*** | | | |
| E1 | ISOAT(ntrac) | I10 | Flag for sorption isotherm type;<br>NTRAC must equal 1<br>= 0 No sorption simulated<br>= 1 Linear isotherm<br>= 2 Freundlich isotherm<br>= 3 Langmuir isotherm |
| | IRCTAT(ntrac) | I10 | Flag for first order decay;<br>NTRAC must equal 1<br>= 0 No decay simulated<br>= 1 First order decay simulated |
| ***(Enter lines ES1 through ES13 if IBIO = 1)*** | | | |
| ES1 | Descriptive text | None | "Elec. Acceptor Isotherm Flags" |
| ES2 | ISOAE(nelec) | I10 | Flag for sorption isotherm type:<br>Enter line ES2 NELEC times |
| ES3 | Descriptive text | None | "Hydrocarbon Isotherm Flags" |
| ES4 | ISOAH(nhcar) | I10 | Flag for sorption isotherm type:<br>Enter line ES4 NHCAR times |
| ES5 | Descriptive text | None | "Nutrient Use and Isotherm Flags" |
| ES6 | INUOPT | I10 | Flag for nutrient utilization option<br>= 1 Multiplicative<br>= 2 Minimum nutrient |
| ES7 | ISOAN(nnutr) | I10 | Flag for sorption isotherm type:<br>Enter line ES7 NNUTR times |
| ES8 | Descriptive text | None | "Product Isotherm and Reaction Flags" |
| ES9 | ISOAP(nprod) | I10 | Flag for sorption isotherm type |

| | | | |
|---|---|---|---|
| | IRCTAP(nprod) | I10 | Flag for first order decay reaction:<br>Enter line ES9 NPROD times |
| ES10 | Descriptive text | None | "Daughter Isotherm and Reaction Flags" |
| ES11 | ISOAD(ndaut) | I10 | Flag for sorption isotherm type |
| | IRCTAD(ndaut) | I10 | Flag for first order decay reaction:<br>Enter line ES11 NDAUT times |
| ES12 | Descriptive text | None | "Tracer Isotherm and Reaction Flags" |
| ES13 | ISOAT(ntrac) | I10 | Flag for sorption isotherm type |
| | IRCTAT(ntrac) | I10 | Flag for first order decay reaction:<br>Enter line ES13 NTRAC times |
| E2 | RHOB(nlay) | RARRAY | Bulk density of the porous medium [M $L^{-3}$];<br>Enter a value for each layer |

***(Enter line E3 and E4 if IBIO = 0 and ISOAT(ntrac) >0)***

| | | | |
|---|---|---|---|
| E3 | SP1AT(nlay, ntrac) | RARRAY | First sorption constant<br>Enter a value for each layer; NTRAC must equal 1<br>Linear => SP1AT is the distribution coefficient $K_d$ [$L^3$ $M^{-1}$]<br>Freundlich => SP1AT is the equilibrium constant $K_f$ [variable]<br>Langmuir => SP1AT is the equilibrium constant $K_l$ [$L^3$ $M^{-1}$] |
| E4 | SP2AT(nlay, ntrac) | RARRAY | Second sorption constant<br>Enter a value for each layer; NTRAC must equal 1<br>Linear => SP2AT is not used, but must be entered<br>Freundlich => SP2AT is the exponent *a*<br>Langmuir => SP2AT is the total conc. of sorption sites [M $M^{-1}$] |

***(Enter line E5 and E6 if IBIO = 0 and IRCTAT(ntrac) >0)***

| | | | |
|---|---|---|---|
| E5 | RC1AT(nlay, ntrac) | RARRAY | First order rate constant for the aqueous phase [$T^{-1}$];<br>Enter a value for each layer; NTRAC must equal 1 |
| E6 | RC2AT(nlay, ntrac) | RARRAY | First order rate constant for the sorbed phase [$T^{-1}$];<br>Enter a value for each layer, NTRAC must equal 1 |

***(Enter the remaining lines only if IBIO = 1)***

| | | | |
|---|---|---|---|
| ES14 | Descriptive text | None | "Electron Acceptor Sorption Constants" |
| ***(Enter line ES15 and ES16 if ISOAE(nelec) >0)*** | | | |
| ES15 | SP1AE(nlay, nelec) | RARRAY | First sorption constant: Enter a value for each layer (inner loop) and for each electron acceptor having ISOAE > 0 (outer loop) |
| ES16 | SP2AE(nlay, nelec) | RARRAY | Second sorption constant: Enter a value for each layer (inner loop) and for each electron acceptor having ISOAE > 0 (outer loop) |
| ES17 | Descriptive text | None | "Hydrocarbon Sorption Constants" |
| ***(Enter line ES18 and ES19 ISOAH(nhcar) >0)*** | | | |
| ES18 | SP1AH(nlay, nhcar) | RARRAY | First sorption constant: Enter a value for each layer (inner loop) and for each hydrocarbon having ISOAH > 0 (outer loop) |
| ES19 | SP2AH(nlay, nhcar) | RARRAY | Second sorption constant: Enter a value for each layer (inner loop) and for each hydrocarbon having ISOAH > 0 (outer loop) |
| ES20 | Descriptive text | None | "Electron Acceptor Sorption Constants" |
| ***(Enter line ES21 and ES22 ISOAN(nnutr) >0)*** | | | |
| ES21 | SP1AN(nlay, nnutr) | RARRAY | First sorption constant: Enter a value for each layer (inner loop) and for each nutrient having ISOAN > 0 (outer loop) |
| ES22 | SP2AN(nlay, nnutr) | RARRAY | Second sorption constant: Enter a value for each layer (inner loop) and for each nutrient having ISOAN > 0 (outer loop) |
| ES23 | Descriptive text | None | "Product Sorption Constants" |
| ***(Enter line ES24 and ES25 ISOAP(nprod) >0)*** | | | |
| ES24 | SP1AP(nlay, nprod) | RARRAY | First sorption constant: Enter a value for each layer (inner loop) and for each product having ISOAP > 0 (outer loop) |
| ES25 | SP2AP(nlay, nprod) | RARRAY | Second sorption constant: Enter a value for each layer (inner loop) and for each product having ISOAP > 0 |

| | | | |
|---|---|---|---|
| | | | (outer loop) |
| ES26 | Descriptive text | None | "Daughter Sorption Constants" |
| ***(Enter line ES27 and ES28 ISOAD(ndaut) >0)*** | | | |
| ES27 | SP1AD(nlay, ndaut) | RARRAY | First sorption constant:<br>Enter a value for each layer (inner loop) and for each daughter having ISOAD > 0 (outer loop) |
| ES28 | SP2AD(nlay, ndaut) | RARRAY | Second sorption constant:<br>Enter a value for each layer (inner loop) and for each daughter having ISOAD > 0 (outer loop) |
| ES29 | Descriptive text | None | "Tracer Sorption Constants" |
| ***(Enter line ES30 and ES31 ISOAT(ntrac) >0)*** | | | |
| ES30 | SP1AT(nlay, ntrac) | RARRAY | First tracer sorption constant:<br>Enter a value for each layer (inner loop) and for each tracer having ISOAT > 0 (outer loop) |
| ES31 | SP2AT(nlay, ntrac) | RARRAY | Second tracer sorption constant:<br>Enter a value for each layer (inner loop) and for each tracer having ISOAT > 0 (outer loop) |
| ES32 | Descriptive text | None | "Product Reaction Constants" |
| ***(Enter line ES33 and ES34 IRCTAP(nprod) >0)*** | | | |
| ES33 | RC1AP(nlay, nprod) | RARRAY | First order rate constant for aqueous phase:<br>Enter a value for each layer (inner loop) and for each product having IRCTAP > 0 (outer loop) |
| ES34 | RC2AP(nlay, nprod) | RARRAY | First order rate constant for sorbed phase:<br>Enter a value for each layer (inner loop) and for each product having IRCTAP > 0 (outer loop) |
| ES35 | Descriptive text | None | "Daughter Reaction Constants" |
| ***(Enter line ES33 and ES34 IRCTAD(ndaut) >0)*** | | | |
| ES36 | RC1AD(nlay, ndaut) | RARRAY | First order rate constant for aqueous phase:<br>Enter a value for each layer (inner loop) and for each daughter having IRCTAD > 0 (outer loop) |
| ES37 | RC2AD(nlay, ndaut) | RARRAY | First order rate constant for sorbed phase:<br>Enter a value for each layer (inner loop) and for each daughter having |

IRCTAD > 0 (outer loop)

| | | | |
|---|---|---|---|
| ES38 | Descriptive text | None | "Tracer Reaction Constants" |

***(Enter line ES36 and ES37 IRCTAT(ntrac) >0)***

| | | | |
|---|---|---|---|
| ES39 | RC1AT(nlay, ntrac) | RARRAY | First order rate constant for aqueous phase: Enter a value for each layer (inner loop) and for each tracer having IRCTAT > 0 (outer loop) |
| ES40 | RC2AT(nlay, ntrac) | RARRAY | First order rate constant for sorbed phase: Enter a value for each layer (inner loop) and for each tracer having IRCTAT > 0 (outer loop) |
| ES31 | NITER | I5 | Number of biodegradation time steps per transport time step |
| ES32 | Descriptive text | None | "Electron Acceptor Inhibition Terms" |

***(Enter lines ES33 and ES34 if the total number of EA processes (including methanogenesis) > 1)***

| | | | |
|---|---|---|---|
| ES33 | Descriptive text | None | "Inhibition of [inhibitee]" Enter this line prior to each inhibitor process. |
| ES34 | AKINH(ninh, ninh) | F10.0 | Electron acceptor inhibition coefficient: Enter AKINH(lj, lk) for each inhibitor *lk* (inner loop) of electron acceptor process *lj* (outer loop) Note that electron acceptor process *lj* will require entry of (*lj* - 1) inhibitors NINH = the total number of electron acceptors processes minus one |

**Example 1: Simulate aerobes and $NO_3$ reducers (NINH = 1)**

Line 1: "Inhibition of $NO_3$"
Line 2: AKINH(1,1) -- coef. of $O_2$ inhibition of $NO_3$

**Example 2: Simulate aerobes, Fe(III), $SO_4$ reducers, and methanogens (NINH = 3)**

Line 1: "Inhibition of Fe(III)"
Line 2: AKINH(1,1) -- coef. of $O_2$ inhibition of Fe(III)

Line 3: "Inhibition of $SO_4$ "
Line 4: AKINH(2,1) -- coef. of $O_2$ inhibition of $SO_4$
Line 5: AKINH(2,2) -- coef. of Fe(III) inhibition of $SO_4$

Line 6: "Inhibition of methanogenesis"
Line 7: AKINH(3,1) -- coef. of $O_2$ inhib. of methanogenesis
Line 8: AKINH(3,2) -- coef. of Fe(III) inhib. of methanogenesis

Line 9: AKINH(3,3) -- coef. of $SO_4$ inhib. of methanogenesis

| | | | |
|---|---|---|---|
| ES35 | Descriptive text | None | "$CH_4$ Inhibition of Methanogenesis" |
| ***(Enter line ES36 if methanogenesis is simulated)*** | | | |
| ES36 | ACH4INH | F10.0 | $CH_4$ Inhibition coefficient: |
| ES37 | Descriptive text | None | "Elec. Acc. Product Generation Coefs." |
| ***(Enter line ES38 if NENDE > 0)*** | | | |
| ES38 | ENDE(nende) | F10.0 | Electron acceptor product generation coefficient:<br>Enter line ES38 NENDE times<br>NENDE is the number of products from the electron acceptors (specified in ENDOPT of the basic transport package). |
| ES39 | Descriptive text | None | "Methane Generation Coefficients" |
| ***(Enter line ES40 if methanogenesis is simulated)*** | | | |
| ES40 | ENDH(nhcar) | F10.0 | Methane generation coefficients:<br>Enter line ES40 NHCAR times |
| ES41 | Descriptive text | None | "Daughter Generation Coefficients" |
| ***(Enter line ES42 if NDAUT >0)*** | | | |
| ES42 | ENDD(ndaut) | F10.0 | Daughter generation coefficients:<br>Enter line ES42 NDAUT times |
| ES43 | Descriptive text | None | "Electron Acceptor Use Coefficients" |
| ES44 | AGAM(nhcar, neatot) | F10.0 | Use coefficients:<br>Enter line ES44 for each hydrocarbon (inner loop) and for electron acceptor (outer loop)<br>Electron acceptor loop is read in the following order: $O_2$, $NO_3$, Fe(III), Mn(IV), $SO_4$ (i.e. from highest to lowest energy).<br>NEATOT is the total number of electron acceptors simulated. Lines are not read for electron acceptors that are not included in the simulation |
| ES45 | Descriptive text | None | "Nutrient Use Coefficients" |
| ***(Enter line ES46 if NNUTR > 0)*** | | | |
| ES46 | APSI(nhcar, nnutr) | F10.0 | Nutrient use coefficients:<br>Enter line ES46 for each hydrocarbon |

(inner loop) and for each nutrient (outer loop)

***(Enter lines ES47 through ES55 NCLNY times:***
***microbial populations will be read in the order of highest to lowest energy)***

| | | | |
|---|---|---|---|
| ES47 | Descriptive text | None | Microbial Population Name, e.g. "Aerobes" |
| ES48 | Descriptive text | None | "Death Rate" |
| ES49 | XKD | F10.0 | First order decay rate for the microbial population<br>XKD < 0 death rate calculated by model (recommended)<br>XKD = 0 no microbial death<br>XKD > 0 death rate is constant at the specified value |
| ES50 | AKHALFH(nhcar, nli, nclny) | F10.0 | Hydrocarbon half saturation constant:<br>Enter line ES50 for each electron acceptor utilized by the microbes (inner loop) and for each hydrocarbon (outer loop)<br>NLI is the number of electron acceptors utilized by the microbes:<br>NLI = 2 for $NO_3$ reducers<br>NLI = 1 for all other populations |

***(Do not enter line ES51 for Fe(III) or Mn(IV) reducers)***

| | | | |
|---|---|---|---|
| ES51 | AKHALFE(nli, nclny) | F10.0 | Electron acceptor half saturation constant:<br>Enter line ES51 for each electron acceptor utilized by the microbes |

***(Enter line ES52 if NNUTR > 0)***

| | | | |
|---|---|---|---|
| ES52 | AKHALFN(nnutr, nli, nclny) | F10.0 | Nutrient half saturation constant:<br>Enter line ES52 for each electron acceptor utilized by the microbes (inner loop) and for each nutrient (outer loop) |

***(Enter line ES53 if STOCHOPT(1) is".true." -- see line AS2)***

| | | | |
|---|---|---|---|
| ES53 | VSPMAX(ncol, nrow, nlay, nhcar, nli, nclny) | RARRAY | Maximum specific rate of substrate utilization:<br>Enter VSPMAX(ncol, nrow) for each layer (inner loop), each electron acceptor utilized by the microbes (middle loop), and for each hydrocarbon (outer loop) |

***(Enter line ES54 if STOCHOPT(1) is".false." -- see line AS2)***

| | | | |
|---|---|---|---|
| ES54 | VSPMAX(nhcar, nli, nclny) | F10.0 | Maximum specific rate of substrate utilization: |

| | | | |
|---|---|---|---|
| | | | Enter line ES54 for each electron acceptor utilized by the microbes (inner loop) and for each hydrocarbon (outer loop) |
| ES55 | YIELD(nhcar, nli, nclny) | F10.0 | Yield coefficients:<br>Enter line ES55 for each electron acceptor utilized by the microbes (inner loop) and for each hydrocarbon (outer loop) |

### *A.2.6 Input Instructions for the NAPL Dissolution Package*

This input file must be created only if the NAPL Dissolution Package is specified in the Basic Transport Package; i.e., IDISS is set to "1". Input is read on unit 22.

Normally, the number of hydrocarbon substrates in the NAPL (NHDIS) will correspond to the number in the overall simulation (NHCAR). However, it is possible to have NHCAR > NHDIS, since contaminants may derive from sources other than the NAPL. Estimates of the initial mass fractions within the NAPL may be obtained from laboratory analysis or from the literature. For example, if the NAPL is gasoline, mass fractions of benzene, toluene, ethylbenzene, and xylenes have been reported (e.g. Sigsby et al., 1987). Values for solubility and molecular weight are readily available from chemical handbooks.

| Line | Variable | Format | Description |
|---|---|---|---|
| FS1 | MXDIS | I10 | Number of nodes where NAPL conc. is specified |
| | IMLOAD | I10 | Flag for mass loading to NAPL:<br>= 0 No time dependent mass loading is simulated<br>= 1 Time dependent mass loading is simulated |
| | NHDIS | I10 | Number of hydrocarbons in the NAPL<br>(0 ≤ NHDIS ≤ NHCAR) |
| | NTDIS | I10 | Number of tracers in the NAPL<br>(0 ≤ NTDIS ≤ NTRAC) |
| ***(Enter the following line only if IMLOAD =1)*** | | | |
| FS2 | NSCH | I10 | Number of schedules for simulation of mass loading |
| | MAXSUB | I10 | Maximum number of subschedules per schedule |
| FS3 | Descriptive text | None | "Initial Mass Fractions of Hydrocarbons" |
| FS4 | FRAH(nhdis) | F10.0 | Initial mass fraction in NAPL:<br>Enter line F4 NHDIS times |
| FS5 | Descriptive text | None | "Initial Mass Fractions of Tracers in NAPL" |
| FS6 | FRAT(ntdis) | F10.0 | Initial mass fraction in NAPL:<br>Enter line F6 NTDIS times |

| | | | |
|---|---|---|---|
| FS7 | Descriptive text | None | "Hydrocarbon Solubility" |
| FS8 | FRAH(nhdis) | F10.0 | Solubility:<br>Enter line F8 NHDIS times |
| FS9 | Descriptive text | None | "Tracer Solubility" |
| FS10 | FRAT(ntdis) | F10.0 | Solubility:<br>Enter line F10 NTDIS times |
| FS11 | Descriptive text | None | "Hydrocarbon Molecular Weight" |
| FS12 | WTMOLH(nhdis) | F10.0 | Molecular weight:<br>Enter line F12 NHDIS times |
| FS13 | Descriptive text | None | "Tracer Molecular Weight" |
| FS14 | WTMOLT(ntdis) | F10.0 | Molecular weight:<br>Enter line F14 NTDIS times |
| FS15 | Descriptive text | None | "Inert Fraction Molecular Weight" |
| FS16 | WTMOLI | F10.0 | Molecular weight |
| FS17 | Descriptive text | None | "NAPL Parameters" |

***(Enter line F18 MXDIS times)***

| | | | |
|---|---|---|---|
| FS18 | KK | I10 | Layer # of block containing NAPL mass |
| | II | I10 | Row # of block containing NAPL mass |
| | JJ | I10 | Column # of block containing NAPL mass |
| | ISCH | I10 | Schedule # for mass loading:<br>Enter any value if IMLOAD = 0 |
| | SINERT | F10.0 | Initial concentration of NAPL [M $M^{-1}$] |
| | DIFALP | F10.0 | Dissolution rate [$T^{-1}$] |
| | TIMEEX | F10.0 | Time when NAPL mass is removed from the block (i.e., excavation). Enter a number larger than the total simulation time to prevent excavation |

***<u>(Enter the remaining lines only if IMLOAD =1)</u>***

| | | | |
|---|---|---|---|
| FS19 | Descriptive text | None | "NAPL Mass Loading" |

***(Enter lines 20 and 21 NSCH times; i.e., for isch = 1 to NSCH)***

| | | | |
|---|---|---|---|
| FS20 | NSUB(isch) | I10 | Number of subschedules in schedule ISCH:<br>1≤ NSUB(isch) ≤ MAXSUB |
| | SCHTIME(isch, 1) | F10.0 | Starting time for NAPL loading according to subschedule 1 |
| | SCHVAL(isch, 1) | F10.0 | Mass rate of NAPL loading according to subschedule 1 [M $T^{-1}$]. |

***(Enter line 21 for isub = 2 to NSUB(isch)***

| | | | |
|---|---|---|---|
| FS21 | SCHTIME(isch, isub) | F10.0 | Starting time for NAPL loading according to subschedule ISUB<br>SCHTIME(isch, nsub(isch) must be greater than the total simulation time |
| | SCHVAL(isch, isub) | F10.0 | Mass rate of NAPL loading according to subschedule ISUB [M $T^{-1}$]. |