Appendix B. SEAM3D Output & Post-Processing

B.1 General Information

The basic output structure for SEAM3D is similar to that of MT3D (Zheng, 1990), and SEAM3D writes output information for all hydrocarbon substrates, electron acceptors, and other constituents in the simulation. The following sections paraphrase and condense information from the MT3D technical documentation (Zheng, 1990), while information relevant to the additional output of SEAM3D is provided in greater detail.

B.2 Output Files

Each time SEAM3D is run, the program generates a standard output file, plus optional output files as requested by the user in the Basic Transport Package (see Section 4.2.1). Options within the Basic Transport Package allow the user to control the frequency and type of information written to the output files. The output files are described below.

1. **Standard Output File (Filename SEAM3D.OUT):**
   This file echoes the input data to allow the user to verify the accuracy of the specified parameters, flags, and options. Each line of input is written to SEAM3D.OUT immediately after being read. If an input error causes the program to stop, the user can find the location of the error by examining SEAM3D.OUT with any text editor. The input error will almost always involve the line that follows the last line successfully written to SEAM3D.OUT. For the times selected by the user, SEAM3D.OUT will contain mass balance information and concentrations of hydrocarbon substrates, electron acceptors (EAs), nutrients, products, daughters, and tracers specified in the simulation.

2. Unformatted Concentration Files:

For each user specified time, these files contain concentrations that can be read by the post-processing programs or used for continuation of a run. If biodegradation is not simulated, then this file is named SEAM3D.UCN, and it contains concentrations of the single contaminant. If biodegradation is simulated, then the following naming system is used:

Model Constituent	File Name		Notes
Hydrocarbon substrates	smh*i*.ucn	*i* = 1, nhcar	nhcar = number of hydrocarbons
Aqueous phase EAs	sme*i*.ucn	*i* = 1, nelec	nelec = number of aqueous EAs
Solid phase EAs	sms*i*.ucn	*i* = 1, nslid	nslid = number of solid phase EAs
Nutrients	smn*i*.ucn	*i* = 1, nnutr	nnutr = number of nutrients
Endproducts	smp*i*.ucn	*i* = 1, nprod	nprod = number of products
Daughters	smd*i*.ucn	*i* = 1, ndaut	ndaut = number of daughters
Tracers	smt*i*.ucn	*i* = 1, ntrac	ntrac = number of tracers

For example, if two hydrocarbon substrates were simulated, then concentrations of the first hydrocarbon would be written to smh1.ucn, and concentrations of the second to smh2.ucn. As another example, if no nutrients were simulated, then there would be no unformatted concentration files written for nutrients.

3. Observation Point Files:

For each user specified observation point, these files contain concentrations versus time in format that can be read by any text editor. If biodegradation is not simulated, then this file is named SEAM3D.OBS, and it contains concentrations of the single contaminant at all observation points. If biodegradation is simulated, then concentrations of all model constituents will be written to an individual file for each observation point. The files are named SMOBS*i*.DAT, for *i* = 1 to the total number of observation points (NOBS). The first line of each SMOBS*i*.DAT file contains a descriptive header that uses the following naming convention:

HC*i* or H*i*	*i*th hydrocarbon substrate
aEA*i*	*i*th aqueous phase electron acceptor
sEA*i*	*i*th solid phase electron acceptor
Nu*i*	*i*th nutrient
Pr*i* or P*i*	*i*th product
Tr*i* or T*i*	*i*th tracer
Mic*i*	*i*th microbial population

Descriptive prefixes may be placed on the header terms. The prefix "Av" indicates a vertically averaged concentration; "Eq" indicates the equilibrium concentration; "Na" indicates the soil concentration of NAPL. The vertically averaged concentration is computed as the average over all model layers of all nonnegative concentrations at the areal location specified by the observation point. Values in the Eq and Na columns will be zero unless the NAPL phase is specified at that observation point. For example, for the first hydrcarbon substrate being simulated, the header term HC1 indicates the substrate concentration, AvH1 indicates the vertically averaged concentration; EqH1 indicates the equilibrium concentration; and NaH1 indicates the NAPL.

4. Total Mass File:

This file, named SMMASS.DAT, contains a time series of the total mass of each constituent in the aqueous, sorbed, and NAPL phases. Total mass is calculated for the entire model domain by summing the mass within each block over the total number of blocks. For the aqueous phase, the mass within each block is the aqueous concentration divided by porosity times the block volume. For the sorbed phase, the mass within each block is the solid phase concentration times bulk density times the block volume. For the NAPL, the mass within each block is the NAPL concentration times bulk density times the block volume. The first line of SMMASS.DAT contains a descriptive header that uses the same abbreviations as in the observation point files, SMOBS*i*.DAT. In addition, suffixes are used on the header terms, with "Aqu" indicating aqueous phase mass, "Ads" indicating adsorbed mass, "NAPL" indicating NAPL mass, and "Tot" indicating the total of the aqueous, adsorbed, and NAPL masses.

5. Mass Balance Summary File:

This file, named SEAM3D.MAS, contains a summary of the mass budget for each constituent simulated.

6. Model Grid Configuration File:

This file, named SEAM3D.CNF, contains information on the spatial discretization to be used by the post-processing program.

6. Transect Output Files:

These files contain concentrations for all model constituents along a transect through the model domain (as specified in the Basic Transport Input file). The format can be read by any text editor. The files are named SMTRN*k*.DAT, for $k = 1$ to the total number of model layers. An additional file named SMTRNAVG.DAT contains vertically averaged concentrations.

6. Contour Output Files:

These files contain concentrations for all model constituents in a format that can be read by contouring graphics packages. The files are named SMSRF*k*.DAT, for $k = 1$ to the total number of model layers. An additional file named SMSRFAVG.DAT contains vertically averaged concentrations.

B.3 Post-Processing

The post-processing programs included with SEAM3D are identical to those of MT3D. The program POSTSM3D uses the unformatted concentrations files (SM*.UCN) and the model grid configuration file (SEAM3D.CNF) to produce data files for plotting. To run POSTSM3D, type the name of the executable file (i.e., "POSTSM3D") at the command prompt, and follow the instructions. Note that POSTSM3D transforms the SEAM3D coordinate system from the upper, top, left corner of block (1, 1, 1) to the lower, bottom, right corner of block 1, NROW, NLAY). Thus the x-axis remains the same, while the y and z-axes are reversed in order to correspond TO the coordinate system of most graphical programs.

The program SAVELAST extracts the last concentrations saved in the SM*.UCN files for use as the starting concentrations for a continuation run (see Appendix A). To run SAVELAST, type the name of the executable file (i.e., "SAVELAST") at the command prompt. The program will prompt for the name of the unformatted concentration file to be read as input and the name of the output file for output.

Since the structure of unformatted files is compiler specific, the user will need to compile PSEAM3D and SAVELAST with same compiler that was used for SEAM3D and MODFLOW. Thus it may be necessary to recompile the source codes PSEAM3D.FOR and SAVELAST.FOR. Additional information on the post-processing programs may be found in the MT3D technical documentation.