

**README File for the
Hydrocarbon Spill Screening Model (HSSM)
Version 1.10
March 1, 1995
Revised April 2, 1996**

1 The Hydrocarbon Spill Screening Model (HSSM) Volume 1 Users' Guide

1.1 Errata

The units for the molecular weights on page 175 should be g/mol and the unit for solubility in equation 45 should be mg/L. This error was corrected in the Adobe pdf file version available at www.epa.gov/ada.

The X2BT.DAT data set contained on the distribution diskette has the value of 4.5 for van Genuchten's n and 2.68 (1/m) for van Genuchten's α (see page 78, Table 27).

Table 114 on page 199 lists the contents of the HSSM-KO data file. Omitted from this listing are the file names. These are found on lines 2 through 8 of the data file. Lines 9-11 are the run title. The input parameters begin on line 12; rather than line 5 as indicated in table 114.

1.2 Answers to Frequently Asked Questions

1.) Can HSSM be used to simulate DNAPL contamination?

Version 1.10 of HSSM is not suited for DNAPLs.

2.) What is the difference between saturation and concentration?

The term saturation is defined as the volume fraction of the pore space that is filled by a given fluid (water, NAPL or air). This term is used only as a measure of the amount of the pore space filled by the fluids. The term concentration is defined as the mass of the chemical constituent per unit volume of water, or in the case of sorbed concentrations as the mass of constituent per unit mass of the solid phase.

If the NAPL fills a fraction of the pore space (saturation), then on a unit volume basis, it is present in much greater mass than if only dissolved in the water (concentration)

3.) Why are there different NAPL/water partition coefficients for a given NAPL?

The NAPL/water partition coefficient (pages 44 and 134, and appendix 3.2) is defined for a given constituent of the NAPL, not the NAPL itself. For example, there is a different value of the NAPL/water partition coefficient for benzene, ethyl benzene, toluene and the xylenes, even though they could all be constituents of the same gasoline (NAPL).

4.) Does HSSM assume there is contamination present before the NAPL release?

In the KOPT portion of HSSM, it is assumed that initially there is no NAPL present in the vadose zone. After passage of NAPL to the water table, NAPL is assumed to be retained in the vadose zone at a saturation equal to the vadose zone residual NAPL saturation.

5.) Which method for estimating the capillary pressure curve parameters should be used?

Three methods are given for determining capillary pressure curve properties in Appendix 3.1. These are the tabulations of Brakensiek et al. (1981) and Carsel and Parrish (1988), and the regression equations of Rawls and Brakensiek (1985). These are all based on near surface soils and may not be representative of aquifers (see Table 93). Each tabulation parameter's have a large standard deviation so that the averages do not necessarily represent the properties of a specific material (see Figure 43). Further, the three methods will not give the same parameter sets for a given texture type.

None of these values are recommended for a specific soil type or aquifer material. The code authors have included these parameter values to prevent model users from putting in completely meaningless values for these parameters. (see page ii).

6.) What property values should be used for diesel fuel?

The following properties for diesel fuel were found in the literature. It should be noted, however, that the composition of diesel fuel is variable and depends upon the source of the crude oil and the methods used in refining (see the paper by Lee et al. that is referenced below). The following may serve as a guide to diesel fuel properties:

Table 1: Diesel Fuels 1-D and 2-D

density	0.80-0.85 g/ml ^(a)
viscosity	1.1 - 3.5 cP @ 40 degrees C ^(a)
surface tension	25 dyne/cm @ 20 degrees C ^(a)
interfacial tension	50 dyne/cm @ 20 degrees C ^(a)
average molecular weight	est. 233 g/mol ^(b)
	^(a) see reference [1]
	^(b) see reference [2]

7) Sometimes increasing the radius multiplication factor does not eliminate the problem in running OILENS.

The radius multiplication factor must be used, because of a singularity in the OILENS equations when the lens radius is equal to the source radius (i.e., at the beginning of the lens spreading). If increasing the radius multiplication factor does not correct the problem, the data set can usually be made to run by including water table fluctuation in the problem. (Water table fluctuation should normally be included in any simulation anyway.)

2 The Hydrocarbon Spill Screening Model (HSSM): Volume 2 Theoretical Background and Source Codes

The input data sets for the sensitivity analysis reported in sections 5 and 6 can be found in the examples directory on the distribution diskette.

3 Version 1.10 Changes to HSSM-KO

In HSSM version 1.10, two corrections have been made to HSSM-KO:

- 1.) When only KOPT is run, the inclusion of a dissolved constituent could cause HSSM-KO to crash. The code has been modified to avoid this problem.
- 2.) Version 1.00 of HSSM would sometimes restrict printing of the front position in the *.HSS file. This problem has been corrected in version 1.10.

4 Version 1.10 Changes to HSSM-T

In HSSM version 1.10, two corrections have been made to HSSM-T:

- 1.) Previously, there was an error in the HSSM-T lens radius, if the percent maximum radius, pmax, input parameter was not set to 101. No error was created if pmax was set to 101 as recommended in the users guide.
- 2.) The input mass flux distribution to HSSM-T is determined from a reduced number of points generated by HSSM-KO. A reduced number of points is used in HSSM-T, because HSSM-KO generates so many output points that the HSSM-T calculations become very slow. Previously the reduction of the number of points may have produced a too-crude input mass flux distribution, if the HSSM-T time step was large. Version 1.10 forces the reduced mass flux distribution to represent the HSSM-KO flux distribution better in these cases

5 Version 1.10 Changes to HSSM-WIN (The Windows Interface)

In the first version of HSSM-WIN (which was designated version 3.1), the values of the van Genuchten parameters alpha and n were displayed reversed. That is the value of n was displayed where alpha should have been and vice versa. This error has been corrected in version 1.1 of HSSM.

The HSSM-WIN interface has been redesignated version 1.10 to match the other parts of HSSM.

5.1 Answers to Frequently Asked Questions

1. When HSSM-KO is executed from the menu immediately after a data set has been edited but not explicitly saved, a box appears which asks:

"Save Current Changes in File"

with choices of Yes, No or Cancel. "Yes" should be selected, if the changes were satisfactory and HSSM-KO should be run.

2. HSSM-WIN saves the directory path with the file names in the HSSM-KO data sets (*.dat). When HSSM is installed or a data set moved from one directory to another, a box appears when the file is opened that says:

"File Needs to be Updated"

"Please Save the File"

followed by the new directory path/file name. The "OK" button should be clicked.

3. To run only KOPT under HSSM-WIN, the "Enable Range Checking" box on the edit menus must be unchecked.

5.2 Windows Installation Procedure for the Windows Version of the Hydrocarbon Spill Screening Model

The procedure described in Volume 1 of the User's Guide for installing HSSM-WIN uses DOS for the installation. The following lists the steps for installation of the Windows version of HSSM using Windows. If the following directions are unclear, check your Windows documentation for more information.

1. Start Windows

(a) Launch Windows by entering the command `win` at the DOS prompt.

2. Copy the HSSM model onto the hard drive (c:).

(a) Locate the Windows File Manager program. *File Manager is usually found in the Main program group. File Manager's icon looks like a filing cabinet.*

(b) Start File Manager by clicking twice on the icon.

- (c) Open a window for the diskette drive (a:) by clicking twice on the drive letter at the top of the file manager window.
- (d) "Tile" the windows by selecting Windows on the file manager menu bar, and then select "tile". (Now the screen should show directories for the hard drive and the diskette drive).
- (e) On drive c: Select the root directory by scrolling up the left hand portion of the window and clicking on c: . (The root directory is the highest level of directory).
- (f) Select File from the File Manager menu bar.
- (g) Select Create directory from this menu.
- (h) In the dialog box type HSSM and click once on the OK button. Check to see that the directory HSSM has been created by scrolling through the directory entries.
- (i) Select the HSSM directory by clicking on HSSM.
- (j) Select the root directory on the a: diskette drive.
- (k) While holding the left mouse button down, drag the mouse to the newly created HSSM directory.
- (l) Release the button and the files will be copied.
- (m) Close the File Manager.

3. Install the HSSM program

- (a) Within Program Manager:
 - i. Select File on the Program Manager menu bar.
 - ii. Select New from this menu.
 - iii. Select Program Group.
 - iv. Enter HSSM Model in the dialog box for the Description.
 - v. Again select File on the Program Manager menu bar.
 - vi. Select New from this menu.
 - vii. Select Program Item.
 - viii. Enter HSSM in the dialog box for the Description.
 - ix. Enter c : \HSSM\HSSM-WIN . EXE for the Command line.

4. Click twice on the icon to execute HSSM.

6 Version 1.10 Changes to the DOS preprocessor PRE-HSSM

The PRE-HSSM preprocessor has been modified to allow entry of the n and alpha van Genuchten parameters.

7 Version 1.10 Changes to the Utility Programs

7.1 RAOULT

Nonzero solubilities need be entered only for NAPL constituents for which partition coefficients are to be calculated.

The full suite of constituents must be entered into RAOULT for either form of the RAOULT calculation (equation 44 or equation 45). For calculation using the average molecular weight, use equation 45 directly.

The name of the RAOULT data set has been changed from RAOULT.DAT to RAOULT.RLT. The new name avoids conflict with HSSM-KO input data sets which have the extension .DAT.

7.2 NTHICK

Sometimes HSSM-KO places the *.NTH file that is required by NTHICK in the root directory (C:) instead of in the current directory.

7.3 NTHICK2

NTHICK2 is a utility that is designed to perform the calculation that is described in Appendix 7 of the HSSM user's guide. NTHICK2 automates the set of steps described in section 7.1 of the appendix.

7.3.1 Notes on NTHICK2

The user should verify that HSSM-KO executes correctly with a trial data set before attempting to run NTHICK2. A trial value of the parameter Somax (say 0.50) can be used; NTHICK2 will later

modify this value. If no lens forms during the HSSM-KO simulation, there is no need (nor possibility) of running NTHICK2.

After verifying that the HSSM-KO data set is correct, NTHICK2 may be run. NTHICK2 will attempt to determine the appropriate value of Somax by running HSSM-KO and performing the calculations that are contained in the original NTHICK.EXE utility. A maximum of ten iterations will be attempted. The procedure used in NTHICK2 (Appendix 7.1) usually converges in 4 or 5 iterations.

When NTHICK2 has completed, the original HSSM-KO input data set will have been modified. The new value of Somax will be contained in the input data set. Also, it is not necessary to run HSSM-KO again, as in running NTHICK2 the complete set of HSSM-KO results are produced. The user may proceed directly to running HSSM-T.

NTHICK2 uses a slightly modified version of HSSM-KO. Therefore the HSSM-KO.EXE file on this diskette must be used with NTHICK2.

NTHICK2 produces input data sets that are incompatible with HSSM-WIN, therefore the DOS interface should be used.

The return key can be pressed repeatedly in order to avoid having to babysit the program as it runs.

If the NTHICK2 procedure fails on a correct HSSM-KO data set please contact Dr. Jim Weaver at 405-436-8545.

References

- [1] J.W. Mercer and R. M. Cohen. A review of immiscible fluids in the subsurface: Properties, models, characterization and remediation. *Journal of Contaminant Hydrology*, 6:107–163, 1990.
- [2] L.S. Lee, M.Hagwall, J.J. Delfino, and P.S.C. Rao. Partitioning of polycyclic aromatic hydrocarbons from diesel fuel into water. *Environmental Science and Technology*, 26(11):2104–2110, 1992.