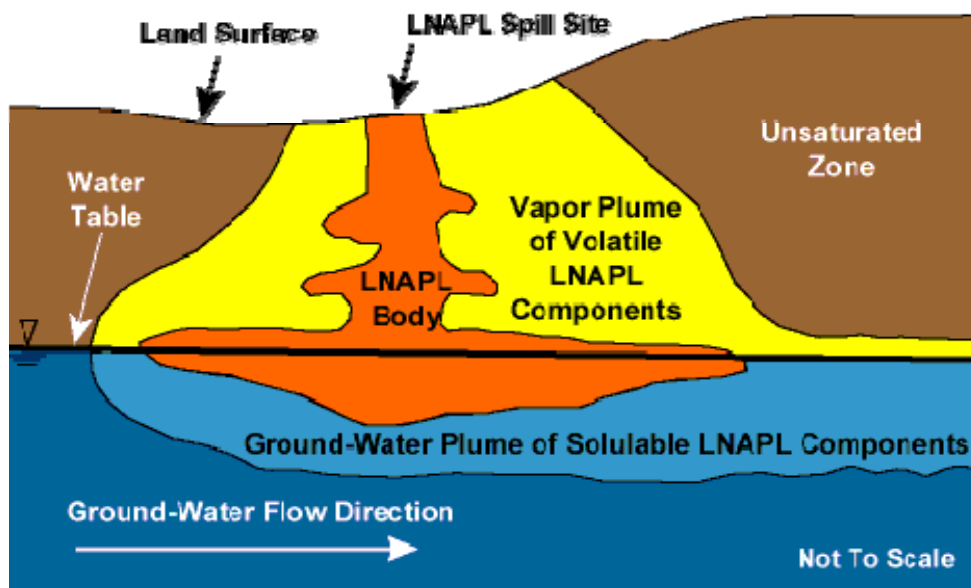


MT3DMS, A Modular Three-Dimensional Multispecies Transport Model – User Guide to the Hydrocarbon Spill Source (HSS) Package

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MT3DMS, A Modular Three-Dimensional Multispecies Transport Model – User Guide to the Hydrocarbon Spill Source (HSS) Package

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Cover image courtesy of Delin, G.N., H.I. Essaid, I.M. Cozzarelli, M.H. Lahvis, and B.A. Bekins. 1998. Ground water contamination by crude oil near Bemidji, Minnesota, USGS Fact Sheet 084-98, U.S. Geological Survey, Reston, VA.

PREFACE

The Hydrocarbon Spill Source (HSS) Package documented in this report provides a seamless linkage to the MT3DMS transport simulator (Zheng and Wang, 1999; Zheng, 2010) for the Hydrocarbon Spill Screening Model (HSSM) (Weaver, 1996). HSSM is a computer code that simulates the vertical migration of a light non-aqueous phase liquid (LNAPL) contaminant through the unsaturated zone and the formation of an oil lens on the water table. It also determines the rate of contaminant mass flux dissolved from the LNAPL source into groundwater. Through the HSS package, the effect of one or more such LNAPL sources is incorporated into 3-D advective-dispersive-reactive transport simulation using MT3DMS Version 5.3 or later. In addition, the HSS package can be used to accommodate any user-defined time-varying mass-loading sources in MT3DMS simulations. Readers of this report are referred to Weaver (1996) for details on the full simulation capabilities of the HSSM suite of programs, and in particular those of the HSSM-KO program, which are unchanged by the linking of codes described in this report. The source code for MT3DMS Version 5.3, including the new Hydrocarbon Spill Source (HSS) Package and associated utilities, is available for download from the website <http://hydro.geo.ua.edu/MT3D>.

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1. INTRODUCTION

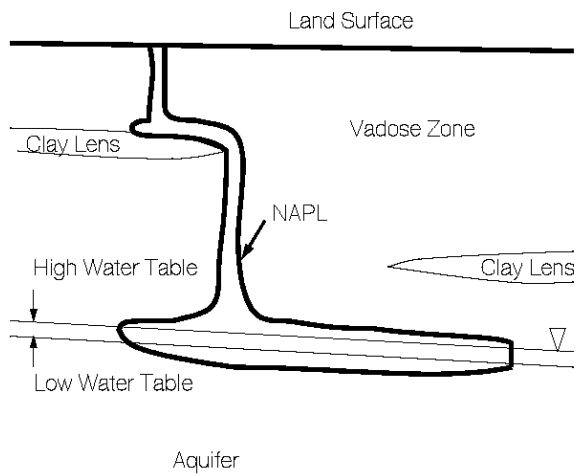
Leaks of fuels that release contaminants such as BTEX, MTBE and other fuel oxygenates are a widespread cause of groundwater contamination throughout the United States. Assessment of the fate and transport of these chemicals requires simulation of the role of the transport of the free-phase light non-aqueous phase liquids (LNAPLs) and their dissolution into the actively flowing groundwater (see Figure 1). A number of computer models have been developed to assess the fate and transport of petroleum hydrocarbon contamination from fuel leaks. However, few of these have included the transport of the free phase contaminants from the vadose (unsaturated) zone to the saturated subsurface under a wide range of hydrogeologic conditions in the field.

The Hydrocarbon Spill Screening Model (HSSM) (Weaver et al., 1996) is a screening-level analytical code developed to estimate the impacts of LNAPLs on water-table aquifers. The model is particularly suited to storage tanks spills and leaks. The model is based on approximate treatments of flow through the vadose zone, LNAPL spreading upon the water table, and miscible transport of a single chemical constituent through a water-table aquifer. HSSM includes two parts: *HSSM-KO* and *HSSM-T*. The HSSM-KO program is comprised of the Kinematic Oily Pollutant Transport (KOPT) module to simulate vadose zone flow and transport of the LNAPL, and the OILENS module to simulate radial spreading and dissolution of the LNAPL at the water table. In general terms, using HSSM the spill of the LNAPL contaminants may be simulated in four ways:

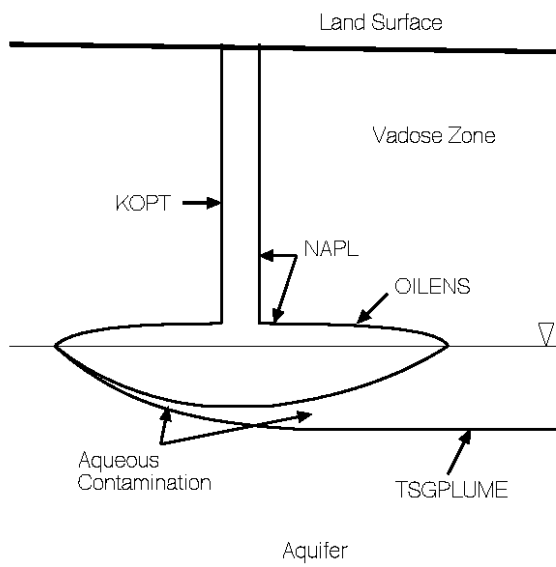
- A known constant flux of LNAPL for a specified duration
- A known volume per unit area of LNAPL placed over a specified depth interval
- A specified constant depth of ponded LNAPL for a certain duration
- Variable ponding after a period of constant head ponding

The output from HSSM-KO is a time-variable mass flux from the free-phase LNAPL spreading lens into the saturated groundwater beneath. The size of the spreading lens is defined by a circular geometry with a time-dependent radius. The rate of dissolution from the free phase into the groundwater in the unit of mass per area is computed by HSSM-KO. The dissolved mass provides the source for the solute transport in the aquifer.

The HSSM-T part of HSSM is comprised of the Transient Source Gaussian Plume Model (TSGPLUME) module for simulating transport of a single miscible species that has dissolved from the LNAPL source. The analytical treatment of the advection-dispersion transport equation executes rapidly, however, the underlying assumptions such as infinite domain and aquifer homogeneity are restrictive. Readers of this report are referred to Weaver et al. (1996) for detailed information on the full simulation capabilities of the HSSM suite of programs, and in particular the simulation capabilities of the HSSM-KO program.



(a)



(b)

Figure 1. (a) Schematic view of contaminant release as a light non-aqueous phase liquid (LNAPL) through the vadose zone and spreading on a water table of an unconfined aquifer and (b) idealized representation of LNAPL release and spreading by the HSSM model components (after Weaver et al., 1996).

This report describes the linking of the MT3DMS transport model with HSSM-KO through the development of a new package for MT3DMS referred to as the Hydrocarbon Spill Source (HSS) Package. In essence, the HSSM-KO program is restructured as a Dynamic Link Library (DLL) that can be called from the MT3DMS main program. The output from HSSM-KO provides a mass-loading source for MT3DMS whose impact on the water-table aquifer can be simulated by MT3DMS under general hydrogeologic conditions. Thus the Transient Source Gaussian Plume Model (TSGPLUME) in the original HSSM code is replaced by the general advection and dispersion solvers available in MT3DMS.

Although the HSS package is intended for use with one or more LNAPL sources generated by the HSSM model, the program design is sufficiently flexible to allow any arbitrarily defined mass-loading sources for MT3DMS. In other words, the user may construct an external input file to represent an arbitrary source for MT3DMS. The external input file contains a set of user-specified time-varying mass-loading rates for any particular source as required by a simulation.

The remainder of this report is organized as follows. Following this introduction in Section 1, Section 2 describes the numerical approach adopted for coupling the codes. Section 3 provides a description of the program design for the HSS package. Section 4 provides detailed input instructions. Section 5 demonstrates the application of the linked codes for simulating two synthetic spill scenarios.

2. NUMERICAL IMPLEMENTATION

Modification to the Finite-Difference Equations

To take full advantage of the capabilities of HSSM-KO and MT3DMS, the two programs have been linked through an implicit formulation. That is, for each transport step in the aquifer, the location and (potentially time-varying) rate of dissolved mass loading from an LNAPL source into the aquifer as determined by the HSSM-KO module is inserted by the HSS package directly into the MT3DMS matrix equations that account for the contribution to mass fluxes from various MT3DMS source terms. The mass-loading sources defined by the HSS package are then solved implicitly along with all other source and sink stresses using the Generalized Conjugate Gradient (GCG) matrix solver as part of the MT3DMS code. With the implicit formulation, there is no transport stepsize limitation on the accommodation of different source strengths.

The general finite-difference equation for the three-dimensional advective-dispersive-reactive transport is derived in the MT3DMS documentation as (Zheng and Wang, 1999):

$$\begin{aligned}
 & A_{i,j,k}^1 C_{i,j,k}^{n+1} + A_{i,j,k}^2 C_{i,j,k-1}^{n+1} + A_{i,j,k}^3 C_{i,j,k+1}^{n+1} + A_{i,j,k}^4 C_{i-1,j,k}^{n+1} + A_{i,j,k}^5 C_{i+1,j,k}^{n+1} + A_{i,j,k}^6 C_{i,j-1,k}^{n+1} \\
 & + A_{i,j,k}^7 C_{i,j+1,k}^{n+1} + A_{i,j,k}^8 C_{i-1,j,k-1}^{n+1} + A_{i,j,k}^9 C_{i,j-1,k-1}^{n+1} + A_{i,j,k}^{10} C_{i,j+1,k-1}^{n+1} + A_{i,j,k}^{11} C_{i+1,j,k-1}^{n+1} \\
 & + A_{i,j,k}^{12} C_{i-1,j,k+1}^{n+1} + A_{i,j,k}^{13} C_{i,j-1,k+1}^{n+1} + A_{i,j,k}^{14} C_{i,j+1,k+1}^{n+1} + A_{i,j,k}^{15} C_{i+1,j,k+1}^{n+1} + A_{i,j,k}^{16} C_{i,j-1,k-1}^{n+1} \\
 & + A_{i,j,k}^{17} C_{i-1,j+1,k}^{n+1} + A_{i,j,k}^{18} C_{i+1,j-1,k}^{n+1} + A_{i,j,k}^{19} C_{i+1,j+1,k}^{n+1} = b_{i,j,k}
 \end{aligned} \tag{1}$$

where C denotes the dissolved concentration, A is the coefficient matrix, and b is the right-hand-side vector containing all known quantities. The 19 coefficients in the coefficient matrix A and the entries in the known right-hand-side vector b are given in Zheng and Wang (1999).

The contribution to the right-hand-side vector of equation (1) from one or more HSS sources can be expressed as follows:

$$b_{i,j,k} = b_{i,j,k} - q_{c(i,j,k)}^n \tag{2}$$

where the term $q_{c(i,j,k)}^n$ is the mass loading rate of the HSS sources at time step n and model cell (i, j, k) [MT^{-1}]. The time-dependent mass loading rates of any HSS source are computed by the HSSM-KO module and saved in a “source definition file” (see the description of this file in “Input Instructions”). The mass loading rate at any arbitrary time, t , between any two HSSM time steps (say, T1 and T2), is obtained from a linear interpolation of the mass loading rates at T1 and T2. **If there are multiple HSSM time steps between the beginning (time1) and ending (time2) of a transport step, a time-averaged mass loading rate over the multiple HSSM time steps is computed and used in equation (2).**

Distribution of Mass Loading among Finite Difference Cells

LNAPL that pools at the water table is simulated by the HSSM-KO module as exhibiting a circular geometry, which can be described by Cartesian center coordinates and a (possibly time-variable) radius. The block-centered finite difference cells used for spatial discretization in MODFLOW and MT3DMS models are four-sided and rectilinear. The cells may or may not have sides of equal length. Note that in developing the HSS package for Version 5.2 of MT3DMS, the center of the HSS source is assumed to be at the center of the active finite difference cell in which it is located (Figure 2).

As long as the circumference of the lens does not cross a cell boundary the full LNAPL lens remains within a single finite difference cell (Figure 2a), and the full mass-loading rate simulated with HSSM-KO (or manually defined by the user) is applied to the single finite difference cell in which it is located. If the circumference of the lens circle crosses one (or more) cell boundaries then the mass must be allocated amongst these cells (Figure 2b). In determining how to allocate the mass amongst multiple cells, two particular objectives must be met:

- The mass must be conserved – i.e. the mass loading calculated by the HSSM-KO module must match the mass influx used for MT3DMS.
- The allocation of mass influx among cells should be a numerically continuous (i.e., a continuously differentiable) process. This ensures that parameter estimation algorithms based on sensitivity calculations obtain accurate and continuous sensitivities for the parameters of HSSM-KO.

To accomplish these objectives an area-weighting approach has been adopted. For simplicity, the discussion below describes the situation of a single HSS source, however, the approach extends logically to multiple sources. When the radius of the lens is greater than the half-width of the cell in either direction, the lens is considered to have crossed a cell boundary. MT3DMS flags that the new cell is an active HSS source, and a three-step mass-allocation algorithm executes:

- The perimeter of the lens is discretized into (i.e., described numerically as) a polyline, with radius equivalent to the lens radius, and with the perimeter represented by a certain number of discrete points.
- The area of overlap of the lens with any finite-difference model cell is calculated. This is accomplished by subdividing a finite-difference cell into a sub-grid. If the nodal center of a sub-cell is inside the radius of the lens, the sub-cell is considered to be part of the overlapped area.
- The area-weighted mass-flux is determined for each cell that is either entirely contained within or overlapping with the lens, as the area of the lens overlapping with (contained within) the cell multiplied by the mass flux per unit area.

In the procedure described above, it is necessary to set the number of discrete points (NPOINT) to approximate the perimeter of the LNAPL lens, and the numbers of columns and rows of a sub-grid to discretize a single finite-difference model cell. By default, NPOINT is set equal to 51 and the numbers of sub-grid columns and rows are both set equal to 25 (NSUBGRID = 25). These default values can be modified in the subroutine HSS5RP.

Larger values lead to more accurate results in computing the areas of the finite-difference model grid that overlap with the LNAPL lens, but at the expense of longer computational times. Note that if zero or a negative radius for the LNAPL lens is specified, the above procedure to determine the overlapping area is bypassed. The mass loading source is only specified for the single cell where the source is located.

In the versions of MT3DMS prior to v5.0, the use of the GCG matrix solver is optional. However, because the HSS package incorporates the LNAPL source term implicitly through the MT3DMS matrix equations, the GCG solver must be selected when the HSS package is active. Failure to do so means that the mass loading from the LNAPL source is not added into the matrix equations. Note that if the HSS package is implemented on MT3DMS after v5.0, the use of the GCG solver is required for all simulations regardless. Finally, it should be pointed out that artifacts may arise from specifying a finite-difference grid spacing that is significantly larger than the (possibly time-varying) lens radius. In this case, numerical ‘spreading’ of the plume (in a manner similar but not analogous to numerical dispersion) may result in a wider dissolved plume that exhibits lower peak concentrations. The simulated lens radius with respect to the cell dimensions should be checked to ensure that this is not taking place.

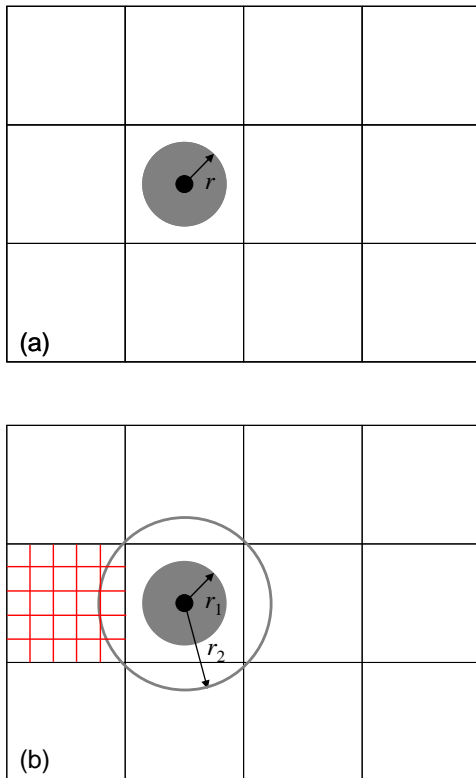


Figure 2. Schematic of the procedure to distribute an LNAPL source into finite-difference model cells: (a) distribution to a single cell when the source perimeter does not cross the cell boundary; and (b) distribution to multiple cells based on the areas of model cells that overlap with the source lens.

3. PROGRAM DESIGN

Implementation of the HSS Package in MT3DMS

The HSS package can be implemented in MT3DMS Version 5.3 or later by inserting the keyword 'HSS' into the transport option array *NameTRNOP* as illustrated below:

```
DATA NameTRNOP/'ADV ', 'DSP ', 'SSM ', 'RCT ', 'GCG ',
&              '      ', '      ', '      ', '      ', '      ',
&              'TOB ', '      ', 'HSS ', '      ', '      ',
&              '      ', '      ', '      ', '      ', '      ',
&              30*'  '/
```

To activate the HSS package, insert a line to the MT3DMS NameFile as shown below:

```
HSS    iunit    input_file_name
```

where **HSS** is the keyword for the HSS package; *iunit* is the input unit number for the HSS package; *input_file_name* is the name of an input file for the HSS package.

An example of the MT3DMS NameFile including the HSS package

```
# MT3DMS 5 Name file for test case test1

# Standard output file
LIST 0 test1.out

# Transport package input files
BTN 0 test1.btn
ADV 0 test1.adv
DSP 0 test1.dsp
SSM 0 test1.ssm
GCG 0 test1.gcg

# HSS package input file
HSS 0 test1.hss

# Flow-Transport Link input file
FTL 0 test1.ftl
```

(Note that unit number 0 is a flag that instructs MT3DMS to use the preset default.)

Description of the HSS Package

The HSS package was written in a modular structure consistent with that of the overall MT3DMS program design. It consists of four primary subroutines: HSS5AL, HSS5RP, HSS5FM, and HSS5BD, where the integer 5 indicates the MT3DMS version number. The functionalities of these subroutines are briefly described below. A simplified flowchart is provided in Figure 3.

HSS5AL

This subroutine allocates memory space for data and working arrays required by the HSS package.

HSS5RP

This subroutine reads input data for the HSS package. It also calls a utility subroutine (GetArea) and two associated functions (INSIDE and CROSS) to determine the areas of finite-difference model cells that overlap with one or more LNAPL source lenses. If the user specifies a flag in the HSS input file to call the HSSM-KO module to generate a 'source-definition file' containing the mass loading rates for each LNAPL source, HSS5RP invokes the dynamic link library 'HSSM-KO.DLL' internally. Otherwise, it is assumed that one or more source-definition files are already available, either by running HSSM externally or created manually for an arbitrary time-vary source.

HSS5FM

This subroutine formulates and adds the HSS source term to the implicit finite-difference equations solved by the GCG matrix solver.

HSS5BD

This subroutine calculates mass budgets associated with the HSS source term.

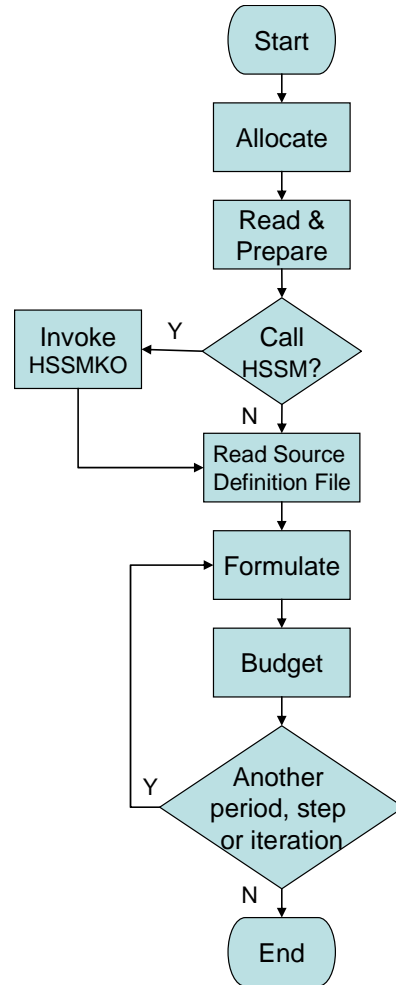


Figure 3. simplified flowchart of the HSS package.

4. INPUT INSTRUCTIONS

Input for the HSS package is read from a file listed in the name file with “HSS” as the file type. The input data are read in free format.

For each simulation

0. [#Text]

Item 0 is optional and can include as many lines as desired. Each line needs to begin with the “#” character in the first column.

1. MaxHSSSource, MaxHSSCells, MaxHSSStep, RunOption
2. faclength, factime, facmass
3. nHSSSource

Read items 4 and 5 [nHSSSource] times

4. HSSFileName, inHSSFile
5. kSource, iSource, jSource, SourceName, iHSSComp

Explanation of Parameters Used by the HSS Package

Text—is a character string (maximum of 79 characters) that starts in column 2. Any characters can be included in [Text]. The “#” character needs to be in column 1. [Text] is printed when the file is read and provides an opportunity for the user to include information about the model both in the input file and the associated output file.

MaxHSSSource—is the maximum number of HSSM-LNAPL sources allowed in the current transport simulation. This value is used only for memory allocation purposes.

MaxHSSCells—is the maximum number of model cells that any single HSSM-LNAPL source can occupy. A HSSM-LNAPL source is initially associated with a single model cell. As the oil lens expands, more model cells may be used to represent the source, whenever necessary. This value is used only for memory allocation purposes.

MaxHSSStep—is the maximum number of time steps used to define any single HSSM-LNAPL source, as output from a HSSM run. This value is used only for memory allocation purposes.

RunOption—is a character flag indicating whether the HSSM model should be invoked from within MT3DMS or run manually outside MT3DMS. If [RunOption] is set to RunHSSM (case insensitive), the HSSM code, included with MT3DMS as a dynamic link library (DLL) module, will be executed from within MT3DMS to simulate the LNAPL source.

If [RunOption] is set to any other value or simply omitted, an input file defining the LNAPL source must have been generated from a previous execution of the HSSM code outside MT3DMS.

faclength—is the conversion factor for converting the unit of length used in HSSM to that used in MT3DMS. For example, if the unit used in MT3DMS is feet while the unit in HSSM is m, [faclength] should be set to 3.28.

factime—is the conversion factor for converting the unit of time used in HSSM to that used in MT3DMS. For example, if the unit used in MT3DMS is minutes while the unit in HSSM is day, [factime] should be set to 1440.

facmass—is the conversion factor for converting the unit of mass used in HSSM to that used in MT3DMS. For example, if the unit used in MT3DMS is gram while the unit in HSSM is kg, [facmass] should be set to 1000.

nHSSSource—is the actual number of HSSM-LNAPL sources included in the current transport simulation. [nHSSSource] cannot exceed [MaxHSSSource], the maximum number of HSSM-LNAPL sources allowed.

HSSFileName—a string of one to 78 nonblank characters specifying the name of an auxiliary input file defining a specific HSSM-LNAPL source. [HSSFileName] can include a path; constraints imposed by a particular computer operating system regarding file names and paths should be considered when specifying [HSSFileName].

inHSSFile—is an integer unit number associated with the HSSM-LNAPL source input file given by [HSSFileName].

kSource—is the layer index of the initial model cell where a HSSM-LNAPL source is located.

iSource—is the row index of the initial model cell where a HSSM-LNAPL source is located.

jSource—is the column index of the initial model cell where a HSSM-LNAPL source is located.

SourceName—is a string of 1 to 12 nonblank characters used to identify the HSSM-LNAPL source specified at [kSource, iSource, jSource]. The identifier need not be unique; however, identification of HSSM-LNAPL sources in the output files is facilitated if each source is given a unique name.

iHSSComp—is species index of the LNAPL source in a multicomponent MT3DMS simulation. For example, if iHSSComp = 2, the LNAPL source is intended for species no. 2 included in the current simulation.

An example of the HSS package input file

```
#
# Input file for the HSS package for MT3DMS
#
# Port Hueneme
# Low-MTBE Gasoline
#

10 5 100 NoRunHSSM /MaxHSSSource, MaxHSSCells, MaxHSSStep, RunOption
1.0 1.0 1.0 /faclength, factime, facmass
1 /nHSSSource
ph-test.dat 33 /HSSFileName, inHSSFile
1 25 25 MTBE 1 /kSource, iSource, jSource, SourceName, iHSSComp
```

Source Definition File

Each HSSM-LNAPL source included in the transport simulation is defined by an input file that has been generated directly by the HSSM code. The content of this input file is listed and discussed below. The input file is arranged in free format and can contain as many lines as necessary. Each input line represents a point on the contaminant mass loading curve computed by HSSM that specifies the rate of mass flux dissolved from the LNAPL source into groundwater (kg/day) and the radius of the oil lenses (m) at different times (days). Note that the time specified in the last input line represents the end of mass loading into groundwater. Thus, if the simulation time for HSSM is shorter than that for MT3DMS, the mass loading rate for the period between the end of HSSM simulation and the end of MT3DMS simulation is considered to be zero.

For each time step computed by the HSSM code:

time, radius_lnapl, sourcemassflux

where

time—is the total elapsed time since the beginning of simulation (unit: day). Note that MT3DMS and HSSM are assumed to have an identical starting time.

radius_lnapl—is the radius of an oil lens developed as a result of a hydrocarbon spill (unit: meter). **If zero or a negative value is assigned to radius_lnapl**, the mass loading source is specified exclusively at the single finite-difference model cell (kSource, jSource, iSource) defined in the HSS input file.

sourcemassflux—is the rate of contaminant mass flux dissolved into groundwater from the LNAPL lenses (unit: kg/d).

An example of the LNAPL source definition file generated by the HSSM code

146.8	7.98	0.00000
147.1	8.29	0.270091E-01
147.5	8.40	0.279162E-01
147.9	8.53	0.289028E-01
148.2	8.63	0.296458E-01
148.6	8.73	0.303775E-01
149.3	8.95	0.320156E-01
150.0	9.17	0.335898E-01
151.1	9.50	0.359083E-01
152.1	9.81	0.381089E-01
153.5	10.19	0.407941E-01
154.9	10.56	0.433267E-01
155.4	10.68	0.441721E-01
155.8	10.78	0.448562E-01
157.3	11.15	0.473079E-01
159.1	11.60	0.503000E-01
161.2	12.08	0.534953E-01
163.5	12.60	0.568072E-01
165.8	13.09	0.599227E-01
168.5	13.64	0.633311E-01
171.2	14.16	0.665323E-01
174.3	14.75	0.700351E-01
177.7	15.36	0.735911E-01
181.0	15.94	0.769179E-01
184.8	16.58	0.804550E-01
188.8	17.22	0.839265E-01
192.9	17.87	0.873066E-01
197.2	18.51	0.905761E-01
201.5	19.14	0.937269E-01
205.9	19.76	0.966709E-01
210.5	20.40	0.996982E-01
215.2	21.03	0.102531
219.9	21.63	0.105154
224.5	22.21	0.107595
227.2	22.48	0.108462
229.7	22.75	0.109445
232.7	23.07	0.110692
235.6	23.40	0.111946
240.9	24.00	0.114231
247.6	24.76	0.117022
254.2	25.49	0.119644

5. TEST PROBLEMS

Problem 1: LNAPL Source in a Uniform Flow Field

In the first test problem, a hypothetical LNAPL source is assumed to leak from the vadose zone and form a circular lens with a constant radius of 7.071 m in a uniform flow field (Figure 4). The mass loading rate of the LNAPL lens is assumed to be 1 kg/day. After 1 year, the LNAPL source is removed and the mass loading rate drops to 0.

A numerical model consisting of 46 columns, 31 rows and 1 layer is constructed for testing the new HSS package. The model grid is so oriented that the flow direction is aligned with model rows. The model parameters used in the test simulation are listed below:

Cell width along rows (Δx) = 10 m
Cell width along columns (Δy) = 10 m
Layer thickness (Δz) = 10 m
Groundwater seepage velocity (v) = 1/3 m/day
Porosity (θ) = 0.3
Longitudinal dispersivity = 10 m
Ratio of transverse to longitudinal dispersivity = 0.3
LNAPL mass loading rate = 1000 g/day for year 1
LNAPL mass loading rate = 0 g/day for year 2
Simulation time (t) = 730 days (2 years)

The flow model is surrounded by specified-head boundaries to the east and west and no-flow boundaries to the north and south. The head values at the specified-head boundaries are arbitrarily chosen to establish the required hydraulic gradient. The transport model is surrounded by zero-mass flux boundaries to the north, south, and west, and specified advective-mass-flux across the east boundary. It is noteworthy that in MT3DMS the dispersive mass flux is assumed to be zero across any boundary by default.

The LNAPL source is specified for the model cell located at row 16, column 16. Because the radius of the LNAPL lens is 7.071 m ($5\sqrt{2}$) and exceeds the half width of the model cell, the LNAPL is distributed into cell (16, 16) and also its four adjacent cells (see the inset of Figure 4). The theoretical values for the partitioning of the source lens among the five model cells should be 63.6% for the central node and 9.1% for the four surrounding cells. The actual values calculated by the HSS package are 64.4%, 8.3%, 8.3%, 9.5%, and 9.5%, respectively. The agreement is reasonable considering the relatively coarse discretization of the source lens perimeter by 51 points and the model cells by a sub-grid of 25 by 25.

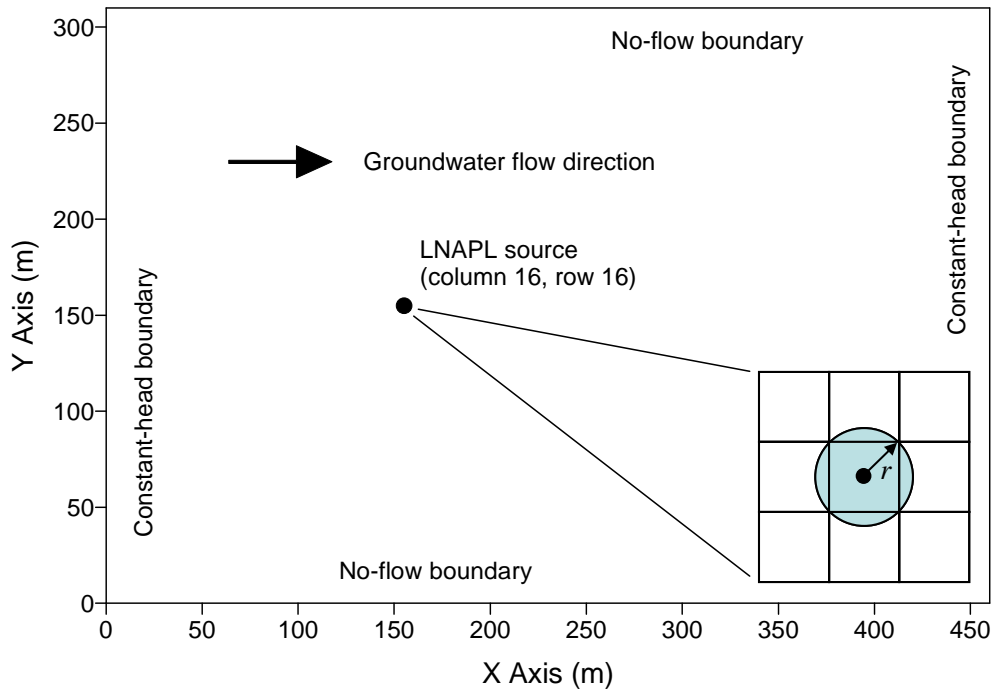


Figure 4. Configuration of the test problem 1.

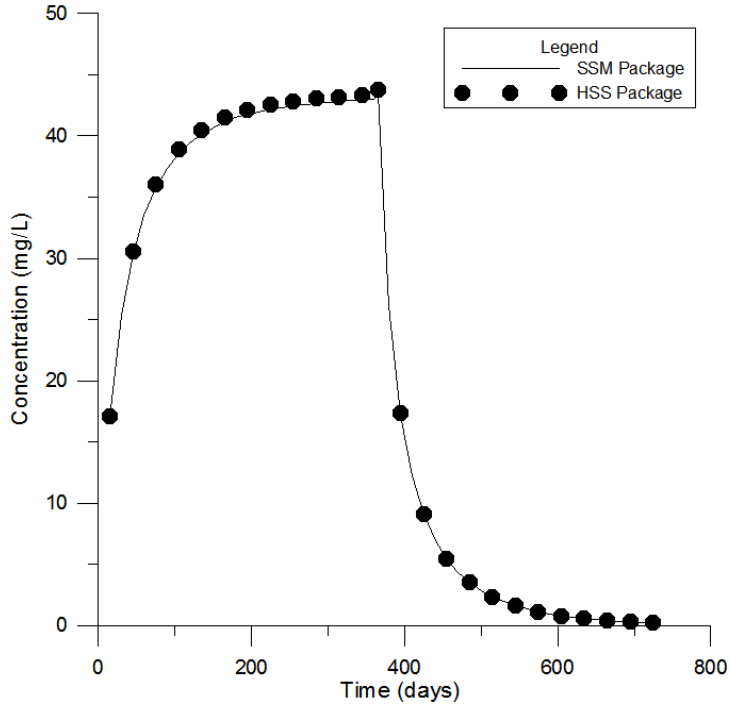


Figure 5. Comparison of the breakthrough curves at the source well as calculated by the originally mass loading option in the SSM package and the new HSS package.

The calculated concentration breakthrough curve at cell (16,16) as calculated by the HSS package is shown in Figure 5 for comparison with that by the mass loading option (type 15) of the original SSM package. For the SSM package, the mass loading rates for each of the five affected cells are specified manually. It can be seen that the agreement is excellent, indicating that the HSS package is capable of handling the automatic partitioning of the LNAPL source into appropriate model cells and the incorporation of the LNAPL source into the implicit finite-difference solution.

Problem 2: Synthetic Field Example

The second test problem is a simplified two-dimensional flow-and-transport simulation based on a hypothetical site with dimensions and hydrogeologic parameters that broadly approximate those of a real-world site. This test problem demonstrates that the new HSS package:

- correctly executes the new HSSM-KO DLL at run-time. The DLL processes two LNAPL sources and writes source definition files tabulating the time-varying dimensions and dissolved mass loading rates from the spreading sources.
- appropriately incorporates the time-varying dissolved mass loading rates into the MT3DMS matrix equations.
- accurately solves the transient mass-transport equations using the implicit GCG solver.

Two hypothetical subsurface releases of gasoline fuel are simulated, each producing an LNAPL lens at the water table that releases dissolved constituents into the actively flowing groundwater (Figure 6). Dissolved phase transport of the fuel oxygenate Methyl Tertiary Butyl Ether (MTBE) is simulated here due to its typically rapid migration in the saturated aquifer compared with other gasoline constituents. Aquifer and transport parameters used for this verification simulation are listed in Table 1.

The model domain is a regular finite difference grid comprising 1 layer, 161 rows and 161 columns. The flow field is maintained constant throughout the simulation using specified-head conditions on the upgradient (right) and downgradient (left) boundaries. The Total-Variation-Diminishing (TVD) scheme is used to solve the advective component of the transport equation to minimize numerical dispersion. The dissolved phase concentration of MTBE is monitored at hypothetical monitoring wells placed downgradient of the first (north) and the second (south) LNAPL sources. The total simulation time is 200 days. The first source is activated at $t = 0.0$ days whereas the second source is activated at $t = 100.0$ days. The HSSM-KO DLL variables specified for both sources are identical, other than the starting time. Both sources produce mass for the duration of the 200-day simulation.

Table 1. Flow and Transport Parameters for Test Problem 2.

Parameter	Value	Units
Hydraulic conductivity	200	ft/day
Recharge rate	1.67	ft/day
Porosity	0.3	
Longitudinal dispersivity	6.63	ft
Transverse dispersivity	0.663	ft

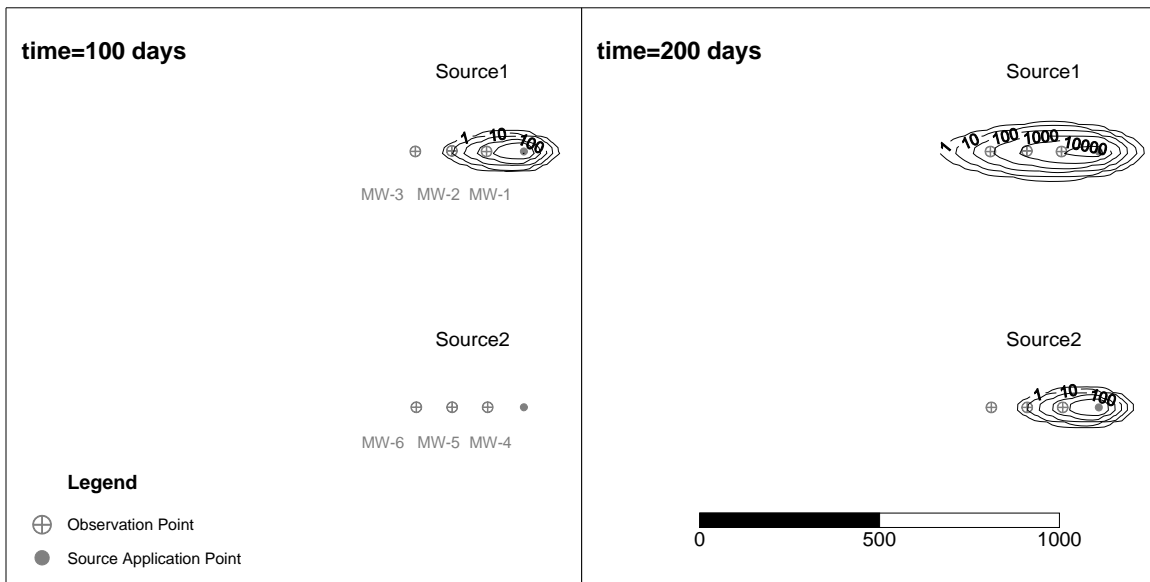


Figure 6. Configuration of the test problem 2 and the simulated plumes from the LNAPL sources 1 and 2 at 100 days (left) and 200 days (right).

Mass loading calculated by the HSSM-KO DLL simulations are 5.730 kg for source no. 1 and 1.233 kg for source no. 2, for a total mass loading of 6.963 kg. The total mass loading calculated by MT3DMS for both sources is 6.987 kg, resulting in a mass balance discrepancy of 0.35%. Figure 7 shows breakthrough curves at the downgradient receptor wells, and profiles of the plume concentrations along their centerline at various times. The results demonstrate that the new HSS package accurately simulates the transfer of mass from the LNAPL lens into the groundwater, and correctly solves the solute transport equation including the new LNAPL sources. The mass balance error can be further reduced by refining the mass loading curve produced by HSSM-KO DLL as read from the source definition file by MT3DMS.

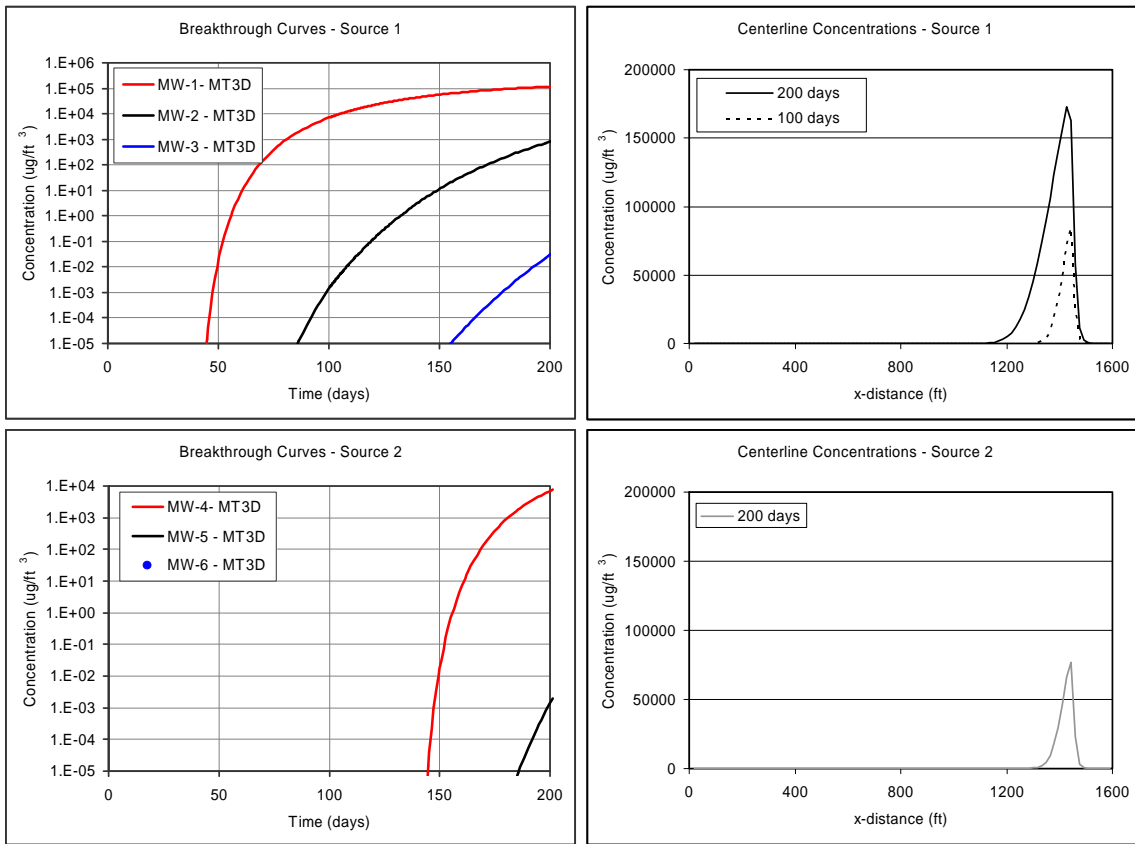


Figure 7. Breakthrough curves at the receptor wells downgradient of sources 1 and 2, respectively (top left and bottom left), and profiles of the plume concentrations along their centerline at various times from sources 1 and 2, respectively (top right and bottom right).

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