



Development of a Density Driven Flow Module for MIKE SHE based on HST3D



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1 Introduction

This document describes the status of the density driven flow module that was developed under the project “Udviklingskontrakt: Videreudvikling af matematisk vandressroucemodelsystem”. The module is based on a commonly accepted density driven flow code developed by the USGS called HST3D. The original code (chapter 2) was adapted in various ways to allow integration with MIKE SHE (chapter 3). In its current state it has been used in a stand-alone application (chapter 4).

2 Short Description of the Original HST3D

The Heat and Solute Transport Program, HST3D (Kipp, 1987) simulates groundwater flow and associated heat and solute transport in three dimensions. The HST3D program may be used for analysis of problems such as those related to subsurface waste injection, landfill leaching, saltwater intrusion, freshwater recharge and recovery, radioactive-waste disposal, hot-water geothermal systems, and subsurface-energy storage. The three governing equations are (1) the saturated groundwater flow equation, formed from the combination of the conservation of total-fluid mass and Darcy's Law for flow in porous media; (2) the heat-transport equation from the conservation of enthalpy for the fluid and porous medium; and (3) the solute transport equation from the conservation of mass for a single-solute species, which may decay and may adsorb onto the porous medium. These are coupled through the dependence of the advective transport on the interstitial pore velocity, the dependence of the fluid density on pressure, temperature and solute-mass fraction and the dependence of the fluid viscosity on temperature and solute mass fraction.

Numerical solutions are obtained for each of the dependent variables: pressure, temperature and mass fraction (solute concentration) in turn. Finite difference techniques are used to discretize the governing equations using a point-distributed grid. The flow and heat and solute transport equations are solved, in turn, after a partial Gauss-reduction scheme is used to modify them. The modified equations are more tightly coupled and have a better stability for the numerical solution.

For the development of a MIKE SHE module, code version 2.05 of HST3D was used. Version 2 of the code (Kipp, 1997) differs from the original code mainly in that (1) the output/input has been improved, (2) there is better handling of unconfined conditions including drying out and re-wetting of cells and (3) reorganisation of the code.

3 Changes to the Original HST3D Required for Incorporation in MIKE SHE

Several changes were made to the original HST3D to make the code (more) suitable for integration in MIKE SHE:

- new top down design for the HST3D program



In this step the subroutines which are now called directly from the main program in HST3D (HST3D.FOR file) are aggregated into intermediate subroutines which can be called from MIKE SHE or another 'driver' program. These new subroutines are:

INIT_HST3D: reading and initialisation for all non-time dependent data

CALC_HST3D: calculate the flow and transport

END_HST3D: cleaning up, closing files, etc.

- dynamic memory allocation
The 2.05 version of HST3D uses common blocks with statically dimensioned arrays. These are replaced by dynamically allocated arrays in f90 modules. Module 'use' statements replace the included metacommands used to insert the common block files in the current source code. During the initialisation in INIT_HST3D the arrays are properly dimensioned using allocation functionality from the modules that contain the array declarations. The 2.05 version of HST3D also uses equivalence statements to allow the same memory to be accessed using different variable names. These equivalence statements degrade the code readability and have been removed or replaced by new array declarations wherever needed.
- block centred grid
HST3D uses a point-distributed grid for discretizing the governing equations while MIKE SHE uses a block-centred grid. To allow integration HST3D was reformulated as a block centred code. This change mainly affects the way the cell properties and the boundaries are handled. In the original point-distributed formulation, cell properties for which values are required at the cell faces (*e.g.* permeability) are defined on an element by element basis. An element is a volume having a node in each of its eight corners and no nodes inside. A cell on the other hand is the volume surrounding a single node for which the faces are the planes halfway between the nodes. By changing to a block-centred discretization, code had to be introduced to calculate cell face values. The input of spatially distributed parameters which was originally on a element basis is now on a cell basis making it possible to use MIKE SHE type input. The implementation of changes to the data reading was done in such a way as to facilitate future shifting from the current MIKE SHE T2 file system to dfs that is used in MIKE ZERO.
- variable layer thickness and topography
In HST3D version 2.05 all layers have constant thickness. For integration of HST3D in MIKE SHE the topography and spatial varying layer thickness was introduced. The user has to specify the topography and the bottom location of each of the model layers as today for the MIKE SHE Saturated Zone (SZ) module. The layer boundaries are used internally in HST3D to calculate the vertical node locations.
- MIKE SHE integration: data exchange and control
The previous modifications were applied to HST3D without requiring any actual integration with MIKE SHE and were tested in a stand-alone application. As a final step, functionality was added to HST3D and MIKE SHE to take care of the data exchange between the two programs.

The first two changes - restructuring of the code and dynamic memory allocation - leave the input for HST3D unchanged and do not affect the results of the program in any way. These changes were therefore tested by comparing output from model runs to the output before any changes were made. For this purpose all available test examples supplied by Ken Kipp were used resulting in a total of 8 tests. Only after these tests were successfully completed the code was changed to block-centred and the topography as well as the variable layer thickness were introduced. The code was then used in an adapted stand-alone HST3D and tested. It is this new adapted stand-alone version and that is described and tested in what follows.



4 A Stand-alone Block-centred HST3D

4.1 Modifications to the HST3D Input

Just as for the original HST3D, all input for the block-centred version is read from a single text file. The following has however been changed in the input file:

- In the original point-distributed formulation the areally distributed cell properties are read on a 'porous medium zone' basis. A 'porous medium zone' is defined as a block of elements an element being the volume having a node in each of its eight corners and no nodes inside. In the new block centred version all 'porous medium zone' related input has been dropped from the HST3D input file and the cell properties are read from MIKE SHE style T2 files with one filename per model layer. Alternatively a constant value can be input instead of a file name.
- Some extra input was added to the file for model area delineation, topography and layer thickness. All this input is read as T2 file names.

By allowing input as T2 files MIKE SHE's graphical input editor can be used to prepare input. The input file is free format and can be freely commented just as for the original HST3D. The general structure of the input file is:

1. title, main dimensions, option flags
2. static data (i.e. non time variant data)
catchment delineation, topography, bottom of layers,
fluid property,
reference condition
solute properties
porous media properties (thermal/solute)
source-sink information (well)
boundary conditions
initial conditions
calculation input (solver)
output selection
3. for each stress period a block of transient data
source-sink (well)
boundary conditions
calculation input (including length of this stress period)
output settings

An example of an input file for one of the test examples is added in addendum A.

4.2 The she2hst Utility

In general, it is a tedious task to prepare the HST3D input file and a utility program (she2hst) was developed which translates the non time variant part of an existing MIKE SHE model to an HST3D input file and the necessary T2 files. She2hst reads its input from a macro file. The HST3D input file produced by she2hst can then, if necessary, be edited to add the solute/heat transport input and/or the time variant input. The file generated by she2hst contains comments indicating where the necessary items should be inserted in the file.



4.3 An Example

4.3.1 Introduction

The intention of this example is both to illustrate how the she2hst and the block centred stand alone HST3D - referred to as BC-HST3D in what follows - can be used as well as, to a limited extent, its correct functioning. The latter is done by comparing the results for the new HST3D with those obtained with the original point distributed version and MIKE SHE (for the groundwater flow test). The example starts out as a simple groundwater model called 'test1'. To this flow model solute is added to arrive at 'test2'.

4.3.2 MIKE SHE model (test1.fsf)

The model domain consists of a square region 400 m x 400 m;
topography is a constant 100 m;
one layer with its bottom at 0m;
horizontal and vertical hydraulic conductivity: 1m/day
specific yield: 0.15
elastic storage coefficient: 0.00001
Initial head condition: 88 m at the left (east) border; 87 m at the right (west) border and 100 m in between.
Boundary conditions: fixed heads at the left and right border; closed boundaries at the bottom and top. This will result in a flow from left (88 m) to right (87 m).

This domain was discretized in the horizontal plane by 100-m squares and in the vertical direction the 100-m thick layer was split into 5 calculation layers of 20-m thickness. This results in a total of 20 calculation compartments. The simulation is run for 1 year.

4.3.3 BC-HST3D setup (test1.hst)

Once the MIKE SHE model (flow setup file; fsf) is completed and the corresponding flow input file (fif) has been generated these can be used by the she2hst program to produce an input file for the BC-HST3D. The input for the she2hst consists of a text file that contains the name of the flow input file for the MIKE SHE setup that needs to be converted i.e. test1.fif:

```
FILETYPE DATATYPE Verno: 10007      0      544
=====
HST3D CONVERTER MACRO FILE
=====
Flow input file      : test1.fif
```

Before the HST3D input file is produced she2hst can be used it has to be edited by the user who needs to specify which output files should be created by HST3D. For this test this is done by changing the output section of the file to:

```
C.3.9.1 .. PRISLM,PRIKD,PRIPTC,PRIDV,PRIVEL,PRIGFB,PRIBCF,PRIWEL; all [I]
1 0 1 1 1 1 1 1
C.3.9.2 .. IPRPTC;(O) - IF PRIPTC [3.9.1] NOT = 0
201
```

The complete input file has been included in appendix A for reference. She2hst also produces the different T2 files referred to in this input file.



4.3.4 Original HST3D model (dat.test1)

When preparing the HST input for this simple example one should take into account the differences between the block centred and the point distributed grid. One difference is that the model boundary passes through the nodes in the point-distributed grid. In the direction of flow (between the specified pressure boundaries) the grid extends from 50 m to 350 m in the horizontal plane. The no-flow boundaries are on the other hand located at 100 m and 300 m. This implies that the grid spacing between the four nodes in the direction perpendicular to flow is not constant but 50 m, 100 m and 50 m. For the vertical direction one extra node needs to be added to the bottom at 0 m to obtain an equivalent point distributed grid for this test case. Also in this direction the grid spacing is irregular so that nodes are located at 0, 10, 30, 50, 70 and 90 m. It should be noted that this grid only will result in the same results as long as the groundwater head is below 90 m as in the point distributed grid the 90 m level is the top boundary of the model domain.

4.3.5 Comparison for test1 MIKE SHE /HST3D/ BC-HST3D

This simple test only involves groundwater flow. As Table 1 shows all these set-ups calculate the same heads, the only difference being the number of digits presented in the results for MIKE SHE compared to both HST3D versions validating the BC-HST3D for this simple test.

Table 1 Heads calculated for the top layer

distance x	MIKE SHE	HST3D	BC-HST3D
0 m	88.00000 m	88.000 m	88.000 m
100 m	87.66807 m	87.668 m	87.668 m
200 m	87.33474 m	87.335 m	87.335 m
300 m	87.00000 m	87.000 m	87.000 m

4.3.6 Solute transport (test2)

Test 1 was extended to solute transport. This was done by setting the associated mass fraction at the left model border to 1. This causes solute to be advected into the model domain at this border. In MIKE SHE the boundary condition for solute is handled in a different way and fixed head cells are treated as fixed concentration cells. Due to this difference the results obtained are shifted one cell as compared to the results for the two HST3D versions and only the results for the two cells between the fixed head cells should be taken into account. Dispersion was included by setting the longitudinal and transverse dispersivity to respectively 100 m and 10 m. Unfortunately, as can be seen from Table 2 the results between the different models differed significantly.

Table 2 Mass fractions calculated for the top layer in the last timestep (NA = not available)

distance x	MIKE SHE	HST3D	BC-HST3D
0 m	0.4794117	0.57660	0.34879
100 m	0.2538109	0.30261	0.13981
200 m	(NA)	0.13156	0.04720
300 m	(NA)	0.07625	0.01095

The results for MIKE SHE are in between those for HST3D and BC-HST3D but this could be due to differences in the numerical solution and the approximation that was made by shifting



the results one cell. However for both HST3D and BC-HST3D the same solver settings were used so the difference in results indicates that there is still an error in the code. Closer analysis of the problem indicates that the difference could at least be partially due to differences in the flows calculated. Although as shown in test1 the heads show a perfect match there is a significant difference in the flows as illustrated in Table 3 and the waterbalance for the BC-HST3D results is unacceptable with its fractional imbalance of 0.4780.

Table 3 Water flows integrated over the boundaries at the end of the simulation

	HST3D	BC-HST3D
Fluid inflow (kg/s)	2.047992E+08	1.967191E+08
Fluid outflow (kg/s)	2.810024E+08	3.487438E+08
fractional imbalance	0.0028	0.4780

5 Conclusions

The intention of the development undertaken for project “Udviklingskontrakt: Videreudvikling af matematisk vandressroucemodelsystem” was to transform HST3D into a module suitable for modelling density driven flow with MIKE SHE. The development effort consisted of five steps of which the first two have been completed successfully. The main issues during the third and fourth steps pertain to changing HST3D from a point-distributed to a block-centred code. This turned out to be a non-trivial task and tests of the current version indicate that more work will be required to obtain a correctly functioning block-centred module. The last step of the development in which the module is added to MIKE SHE has been partially implemented but further testing of the integration has been postponed until the module is shown to function properly in a stand-alone application.

6 Literature

Kipp, K.L., Jr., 1997, Guide to the revised heat and solute transport simulator, HST3D--Version 2: U.S. Geological Survey Water-Resources Investigations Report 97-4157, 149 p.

Kipp, K.L., Jr., 1986, HST3D--A computer code for simulation of heat and solute transport in three-dimensional ground-water flow systems: U.S. Geological Survey Water-Resources Investigations Report 86-4095, 597 p.



Appendix A Block centred HST3D input file generated using she2hst.

```
C HST_SHE Data-Input Form
C Notes:
C Input lines are denoted by C.N1.N2.N3 where
C N1 is the read group number, N2.N3 is the record number
C A letter indicates an exclusive record choice must be made.
C   i.e. A or B or C
C (O) - Optional data with conditions for requirement
C P [n.n.n] - The record where parameter P is set
C Input by x,y,z range format is:
C.0.1.. X1,X2,Y1,Y2,Z1,Z2
C.0.2.. VAR1,IMOD1,[VAR2,IMOD2,VAR3,IMOD3]
C Use as many of line 0.1 & 0.2 sets as necessary
C End with line 0.3
C.0.3.. END OR end
C {nnn} - Indicates that the default number, nnn, is used if a zero
C         is entered for that variable
C [T/F] - Indicates a logical variable
C [I] - Indicates an integer variable
C-----
C-----
C Start of the data file
C Specification and dimensioning data - READ1
C.1.1 .. TITLE Line 1
HST3D style input produced from
C.1.2 .. TITLE Line 2
MIKE SHE setup data for setup :test1.fif
C.1.3 .. RESTRT[T/F],TIMRST
C RESTRT should always be F with SHE use
F /
C.1.4 .. HEAT[T/F],SOLUTE[T/F],EEUNIT[T/F],CYLIND[T/F],SCALMF[T/F]
F F F F F
C.1.5 .. TMUNIT[I] Only code 1 (seconds) allowed with MSHE
1
C.1.6 .. NX,NY,NZ,NHCN
4 4 5 0
C.1.7 .. NSBC,NFBC,NLBC,NETBC,NAIFC,NHCBC,NWEL
1 0 0 0 0 0 0
C.1.8 .. SLMETH[I] default is 5 with MSHE
1
C-----
C-----
C Static data - READ2
C.2.1.. catchment delineation (T2 file name) (K), K =1, NZ
MAPS\test1_ibc_001.T2
MAPS\test1_ibc_002.T2
MAPS\test1_ibc_003.T2
MAPS\test1_ibc_004.T2
MAPS\test1_ibc_005.T2
C.2.2.. Topography (T2 or constant)
MAPS\test1_topo.T2
C.2.3. Bottom of layer (K), K =1, NZ
MAPS\test1_bot_001.T2
MAPS\test1_bot_002.T2
MAPS\test1_bot_003.T2
MAPS\test1_bot_004.T2
MAPS\test1_bot_005.T2
C-----
C-----
C Fluid property information
C.2.4.1 .. BP
0.00000E+00
C.2.4.2 .. P0,T0,W0,DENF0
0.00000E+00 0.10000E+02 0.00000E+00 0.10000E+04
C.2.4.3 .. W1,DENF1;(O) - SOLUTE [1.4]
C.2.4.4 .. VISFAC
-0.10000E-02
C-----
C-----
C Reference condition information
C.2.5.1 .. PAATM
0.00000E+00
C.2.5.2 .. POH,T0H
0.00000E+00 0.10000E+02
C-----
C-----
C Fluid thermal property information
```



```
C.2.6 .. CPF,KTHF,BT;(O) - HEAT [1.4]
C-----
C Solute information
C.2.7 .. DM,DECLAM;(O) - SOLUTE [1.4]
C.2.8 .. NO Porous media zone information with MSHE
C-----
C Porous media property information
C.2.9.1.a KXX(K), K = 1, NZ
MAPS\test1_kxx_001.T2
MAPS\test1_kxx_002.T2
MAPS\test1_kxx_003.T2
MAPS\test1_kxx_004.T2
MAPS\test1_kxx_005.T2
C.2.9.1.b KYY(K), K = 1, NZ
MAPS\test1_kyy_001.T2
MAPS\test1_kyy_002.T2
MAPS\test1_kyy_003.T2
MAPS\test1_kyy_004.T2
MAPS\test1_kyy_005.T2
C.2.9.1.c KZZ(K), K = 1, NZ
MAPS\test1_kzz_001.T2
MAPS\test1_kzz_002.T2
MAPS\test1_kzz_003.T2
MAPS\test1_kzz_004.T2
MAPS\test1_kzz_005.T2
C.2.9.2 .. POROS(K), K = 1, NZ
MAPS\test1_poros_001.T2
MAPS\test1_poros_002.T2
MAPS\test1_poros_003.T2
MAPS\test1_poros_004.T2
MAPS\test1_poros_005.T2
C.2.9.3 .. ABPM(K), K = 1, NZ
MAPS\test1_abpm_001.T2
MAPS\test1_abpm_002.T2
MAPS\test1_abpm_003.T2
MAPS\test1_abpm_004.T2
MAPS\test1_abpm_005.T2
C-----
C Porous media thermal property information
C.2.10.1 .. RCPPM(K), K = 1, NZ ;(O) - HEAT [1.4]
C.2.10.2.a .. KTHXPM(K), K = 1, NZ ;(O) - HEAT [1.4]
C.2.10.2.b .. KTHYPM(K), K = 1, NZ ;(O) - HEAT [1.4]
C.2.10.2.c .. KTHZPM(K), K = 1, NZ ;(O) - HEAT [1.4]
C-----
C Porous media solute and thermal dispersion information
C.2.11.a .. ALPHL(K), K = 1, NZ ;(O) - SOLUTE and/or HEAT [1.4]
C.2.11.b .. ALPHT(K), K = 1, NZ ;(O) - SOLUTE and/or HEAT [1.4]
C-----
C Porous media solute property information
C.2.12 .. DBKD(K), K = 1, NZ ;(O) - SOLUTE [1.4]
C-----
C Source-sink well information
C.2.13.1 .. IWEL,XW,YW,ZWB,ZWT,WBOD,WQMETH[I];(O) - NWEL [1.7] >0
C.2.13.2 .. WCF(L);L = 1 to NZ-1 (EXCLUSIVE) by ELEMENT
C.2.13.3 .. WSF(L);L = 1 to NZ-1 (EXCLUSIVE) by ELEMENT
C.2.13.4 .. WRISL,WRID,WRRUF,WRANGL;(O) - NWEL [1.7] >0 and
C WRCALC(WQMETH [2.13.1] >30)
C.2.13.5 .. HTCWR,DTHAWR,KTHAWR,KTHWR,TABWR,TATWR;(O) - NWEL [1.7] >0
C WRCALC(WQMETH [2.13.1] >30) and HEAT [1.4]
C Use as many sets of 2.13.1-5 lines as necessary for each well
C.2.13.6 .. End with END
C.2.13.7 .. MXITQW{10},TOLDPW{6.E-3},TOLFPW{.001},TOLQW{.001},DAMWRC{2.},
C DZMIN{.01},EPSWR{.001};(O) - NWEL [1.7] >0 and WRCALC(WQMETH[2.13.1] >30)
C-----
C Boundary condition information
C-----
C Specified value b.c.
C.2.14 .. IBC (O) NSBC [1.7] > 0
C.2.14.a.1.. SBCP [T/F] (O) NSBC [1.7] > 0
T
C.2.14.a.2.. T2 Maps with the specified pressure boundary conditions (O) SBCP [2.14.a.1]
MAPS\test1_sbc_001.T2
MAPS\test1_sbc_002.T2
MAPS\test1_sbc_003.T2
MAPS\test1_sbc_004.T2
MAPS\test1_sbc_005.T2
C.2.14.b.1.. SBCT [T/F] (O) NSBC [1.7] > 0 AND HEAT
C.2.14.b.2.. T2 Maps with the specified temperature boundary conditions (O) SBCT [2.14.a.1]
```



```
C.2.14.c.1.. SBCS [T/F] (O) NSBC [1.7] > 0 AND SOLUTE
C.2.14.c.2.. T2 Maps with the specified solute boundary conditions (O) SBCS [2.14.a.1]
C-----
C..... Specified flux b.c.
C.2.15 .. IBC (O) NFBC [1.7] > 0
C.2.15.a.1.. FBCT [T/F] (O) NFBC [1.7] > 0
C.2.15.a.2.. T2 Maps with the flux boundary condition for the water flow
C.2.15.b.1.. FBCT [T/F] (O) NFBC [1.7] > 0 AND HEAT
C.2.15.b.2.. T2 Maps with the flux boundary condition for the heat transport
C.2.15.c.1.. FBCT [T/F] (O) NFBC [1.7] > 0 AND SOLUTE
C.2.15.c.2.. T2 Maps with the flux boundary condition for the solute transport
C-----
C Aquifer and river leakage b.c.
C No Aquifer and river leakage b.c. with MSHE: use the MSHE possibilities for this
C.2.16.1 .. IBC by x,y,z range {0.1-0.3} with no IMOD parameter;(O) -
C NLBC [1.7] >0
C.2.16.2 .. KLBC,BLBC,ZELBC by x,y,z range {0.1-0.3};(O) - NLBC [1.7] >0
C River leakage b.c.
C.2.16.3 .. XR1,YR1,XR2,YR2,KRBC,BBRBC,ZERBC;(O) - NLBC [1.7] > 0
C.2.16.4 .. End with END
C-----
C Evapotranspiration b.c.
C No Evapotranspiration b.c. with MSHE: use the MSHE possibilities for this
C.2.17.1 .. IBC by x,y,z range {0.1-0.3} with no IMOD parameter;(O) -
C NETBC [1.7] >0
C.2.17.2 .. ZLSETB,BETBC by x,y,z range {0.1-0.3};(O) - NETBC [1.7] >0
C-----
C Aquifer influence functions
C No Aquifer influence functions with MSHE
C.2.18.1 .. IBC by x,y,z range {0.1-0.3} with no IMOD parameter;(O) - NAIFC [1.7] > 0
C.2.18.2 .. UVAIFC by x,y,z range {0.1-0.3};(O) - NAIFC [1.7] > 0
C.2.18.3 .. IAIF;(O) - NAIFC [1.7] > 0
C Pot a.i.f.
C.2.18.4A .. ABOAR,POROAR,VOAR;(O) - IAIF [2.18.3] = 1
C Transient, Carter-Tracy a.i.f.
C.2.18.4B .. KOAR,ABOAR,VISOAR,POROAR,BOAR,RIOAR,ANGOAR;(O) - IAIF [2.18.3] = 2
C-----
C Heat conduction b.c.
C No Heat conduction b.c.with MSHE
C.2.19.1 .. ZHCBC(K);(O) - HEAT [1.4] and NHCBC [1.7] > 0
C.2.19.2 .. IBC by x,y,z range {0.1-0.3} with no IMOD parmeter;(O) -
C HEAT [1.4] and NHCBC [1.7] > 0
C.2.19.3 .. DTHHC by x,y,z range {0.1-0.3} for HCBC nodes;(O) -
C HEAT [1.4] and NHCBC [1.7] > 0
C.2.19.4 .. KHCBC by x,y,z range {0.1-0.3} for HCBC nodes;(O) -
C HEAT [1.4] and NHCBC [1.7] > 0
C-----
C Free surface b.c.
C.2.20 .. FRESUR[T/F]
T
C-----
C Initial condition information
C.2.21.1 .. ICHYDP[T/F]
F
C.2.21.2 .. ICHWT[T/F];(O) - FRESUR [2.20]
T
C.2.21.3A .. ZPINIT,PINIT;(O) - ICHYDP [2.21.1] and NOT ICHWT [2.21.2]
C.2.21.3B .. initial P(K), K= 1, NZ {0.1-0.3};(O) - NOT ICHYDP [2.21.1] and
C NOT ICHWT [2.21.2]
C.2.21.3C .. HWT by x,y,z range {0.1-0.3};(O) - FRESUR [2.20] and
C ICHWT [2.21.2]
MAPS\test1_hwt.T2
C.2.21.4 .. T(K), K = 1, NZ {0.1-0.3};(O) - HEAT [1.4]
C.2.21.5 .. NZTPHC, ZTHC(I),TVZHC(I);(O) - HEAT [1.4] and NHCBC [1.7] >0
C NHCBC is 0 with MSHE
C.2.21.6 .. C by x,y,z range {0.1-0.3};(O) - SOLUTE [1.4]
C-----
C Calculation information
C.2.22.1 .. FDSMTH,FDTMTH
0.50000E+00 0.10000E+01
C.2.22.2 .. TOLDEN{.001},MAXITN{5}
0.10000E-02 5
C Two-line s.o.r. solver NOT used with MSHE
C.2.22.3 .. NTSOPT{5},EPSSLV{1.e-7},EPSOMG{.2},MAXIT1{50},MAXIT2{100}
C Generalized, restarted conjugate-gradient solver
C.2.22.4 .. IDIR,IORDER,NSDR,EPSSLV{1.e-5},MAXIT2{100}
C (O) - SLMETH [1.8] = 3 or 5; (always 5 with MSHE but edited here)
C 1 2 6 0.10000E-06 100
```



```
C-----
C Output information
C.2.23.1 .. PRTPMP,PRTFP,PR TIC,PR TBC,PR TSLM,PR TWEL; all [T/F]
F F F F F F
C.2.23.2 .. IPRPTC,PR TDV[T/F];(O) - PR TIC NOT used with MSHE
C.2.23.3 .. ORENPR[I];(O) - NOT CYLIND [1.4]
12
C.2.23.4 .. PLTZON[T/F];(O) - PR TPMP [2.23.1] NOT used with MSHE
C.2.23.5 .. PLTTEM[T/F]
F
C-----
C
C-----
C TRANSIENT DATA - READ3
C.3.1 .. THRU[T/F]
F
C If THRU is true, proceed to record 3.99
C-----
C The following is for NOT THRU
C-----
C Source-sink well information
C.3.2.1 .. RDWTD[T/F];(O) - NWEL [1.7] > 0
C.3.2.2 .. IWEL,QWV,PWSUR,PWK T,TWSRKT,CWKT;(O) - RDWTD [3.2.1]
C Use as many 3.2.2 lines as necessary
C.3.2.3 .. End with END
C-----
C Boundary condition information
C-----
C..... Specified value b.c.
C.3.3.1 .. RDSPBC,RDSTBC,RDSCBC; all [T/F];(O) - NSBC [1.7] > 0
T F F
C.3.3.2 .. PNP B.C. layer number / T2MAP or constant value (O) RDSPBC [3.3.1]
C
end with end
1
MAPS\test1_pnp_001.T2
2
MAPS\test1_pnp_002.T2
3
MAPS\test1_pnp_003.T2
4
MAPS\test1_pnp_004.T2
5
MAPS\test1_pnp_005.T2
END
C.3.3.3 .. TSBC layer number / T2MAP or constant value (O) RDSPBC [3.3.1] and HEAT [1.4]
C
end with end
C.3.3.4 .. CSBC layer number / T2MAP or constant value (O) RDSPBC [3.3.1] and SOLUTE [1.4]
C
end with end
C.3.3.5 .. TNP B.C. layer number / T2MAP or constant value (O) RDSTBC [3.3.1] and HEAT [1.4]
C
end with end
C.3.3.6 .. CNP B.C. layer number / T2MAP or constant value (O) RDSCBC [3.3.1] and SOLUTE
[1.4]
C
end with end
C-----
C Specified flux b.c.
C.3.4.1 .. RDFLXQ,RDFLXH,RDFLXS; all [T/F];(O) - NFBC [1.7] > 0
C.3.4.2 .. QFFXYZ B.C. layer number / T2MAP or constant value (O) RDFLXQ [3.4.1]
C.3.4.3 .. UDENBC layer number / T2MAP or constant value (O) RDFLXQ [3.4.1]
C.3.4.4 .. TFLX layer number / T2MAP or constant value (O) RDFLXQ [3.4.1] and HEAT [1.4]
C.3.4.5 .. CFLX B.C. layer number / T2MAP or constant value (O) RDFLXQ [3.4.1] and SOLUTE
[1.4]
C.3.4.6 .. QHFXYZ B.C. layer number / T2MAP or constant value (O) RDFLXH [3.4.5]
C.3.4.7 .. QSFXYZ B.C. layer number / T2MAP or constant value (O) RDFLXS [3.4.1]
C-----
C Leakage b.c. (Normally NOT used with MSHE)
C.3.5.1 .. RDLBC[T/F];(O) - NLBC [1.7] > 0
C.3.5.2 .. PHILBC,DENLBC,VISLBC by x,y,z range {0.1-0.3};(O) - RDLBC [3.5.1]
C.3.5.3 .. TLBC by x,y,z range {0.1-0.3};(O) - RDLBC [3.5.1] and HEAT [1.4]
C.3.5.4 .. CLBC by x,y,z range {0.1-0.3};(O) - RDLBC [3.5.1] and SOLUTE [1.4]
C-----
C River leakage b.c. (Normally NOT used with MSHE)
C.3.5.5 .. XR1,YR1,XR2,YR2,HRBC,DENRBC,VISRBC,TRBC,CRBC;(O) - RDLBC [3.5.1]
C.....Use as many 3.5.5 lines as necessary
C.3.5.6 .. End with END
C-----
C Evapotranspiration b.c. (Normally NOT used with MSHE)
C.3.6.1 .. RDETBC[T/F];(O) - NETBC [1.7] > 0
C.3.6.2 .. QETBC by x,y,z range {0.1-0.3};(O) - RDETBC [3.5.1]
C-----
```



```
C Aquifer influence function b.c. (Normally NOT used with MSHE)
C.3.7.1 .. RDAIF[T/F];(O) - NAIFC [1.7] > 0
C.3.7.2 .. DENOAR by x,y,z range {0.1-0.3};(O) - RDAIF [3.7.1]
C.3.7.3 .. TAIF by x,y,z range {0.1-0.3};(O) - RDAIF [3.7.1] and HEAT [1.4]
C.3.7.4 .. CAIF by x,y,z range {0.1-0.3};(O) - RDAIF [3.7.1] and SOLUTE [1.4]
C-----
Calculation information
C.3.8.1 .. RDCALC[T/F]
T
C.3.8.2 .. AUTOTS[T/F];(O) - RDCALC [3.8.1]
T
C.3.8.3A .. DELTIM;(O) - RDCALC [3.8.1] and NOT AUTOTS [3.8.2]
C.3.8.3B .. DPTAS{5E4},DTTAS{5.},DCTAS{.25},DTIMMN{1.E4},DTIMMX{1.E7};
C          (O) - RDCALC [3.8.1] and AUTOTS [3.8.2]
      50000      5      0      10000 10000000
C.3.8.4 .. TIMCHG
      0.31536E+08
C-----
C Output information
C Next input only to be used during testing of stand alone MIKE SHE version
C.3.9.1 .. PRISLM,PRIKD,PRIPTC,PRIDV,PRIVEL,PRIGFB,PRIBCF,PRIWEL; all [I]
      1 0 1 1 1 1 1 1
C.3.9.2 .. IPRPTC;(O) - IF PRIPTC [3.9.1] NOT = 0
      201
C.3.9.3 .. CHKPTD[T/F],PRICPD,SAVLDO[T/F]
      F /
C-----
C Contour and vector map information
C.3.10.1 .. CNTMAP[T/F],VECMAP[T/F],PRIMAP[I]
      F F /
C-----
C Read sets of READ3 data at each TIMCHG until THRU (Lines 3.N1.N2)
C-----
C End of simulation line follows, THRU=.TRUE.
C.3.99.1 .. THRU
T
C End of the data file
C-----
C-----
```