MIKE SHE WQ – User Manual

Particle Tracking Module

CONTENTS

1 INTRODUCTION

This document serves as the users manual and technical reference for the MIKE SHE Particle Tracking (PT) module.

PT allows the user to calculate the flow path of a number of hypothetical particles, which are moved in the three-dimensional, saturated groundwater zone (SZ). The particles are displaced individually in a number of time steps. The movement of each particle is composed of a deterministic part, in which the particle is moved according to the local ground water velocity calculated by the MIKE SHE water movement module, and a stochastic part where the particle is moved randomly based on the local dispersion coefficients.

Particle tracking is only calculated for the saturated zone (SZ) and particles that leave SZ are not traced any further. Initially, the user assigns a number of particles to the compartments of the model grid (the computational cells). Input of particles during the calculation can occur from sources in the precipitation or SZ or from boundary or internal constant concentration cells. Particles leave SZ when they arrive at a boundary or an internal constant concentration cell or when they go to a sink. Possible sinks in the Particle Tracking are wells, rivers, drains, and exchange with the unsaturated zone (UZ).

All particles are assigned a mass, which means that a number of particles within a specific volume corresponds to a solute concentration. The Particle Tracking module can therefore be used for solute transport simulations and is in some cases superior to the conventional numerical solution of the advection-dispersion equation since numerical dispersion is negligible. However it is expected that the module will be used mostly for delineation of abstraction well capture zones and upstream zones and for determination of groundwater age and solute transport times, which are some of the features the particle tracking module is offering.

2 ACTIVATING THE MIKE SHE PARTICLE TRACKING MODULE

The PT module can be activated in two ways: by input in the transport setup file (<setupname>.tsf) or by setting an environment variable.

The recommended way to turn on PT is by adding the following line to the end of the transport setup file (<setupname>.tsf):

PARTICLE TRACKING : T

To turn off the Particle Tracking the user should change this line to:

PARTICLE TRACKING : F

Notice: The line should be inserted below the "End of File"-line to stress PT-computation is an external option, see the example in Figure 1.

Alternatively, a possibility in which an environment variable is used is retained in this version for backward compatibility with previous versions of PT.

The environment variable is set by editing the file %shedir%\sheenv.bat to activate the PT module.

The line containing:

```
set ptcalc=off
```

must be changed to

```
set ptcalc=on
```

The PT module will then be executed instead of the finite difference solution of the advection-dispersion equation. If the finite difference solver, i.e. the advection-dispersion module, is preferred the sheenv.bat file should be changed back to its original appearance.

Notice: By setting the environment variable TRUE the PT module will always be executed regardless of the input in the transport set-up file: the PT module is used when either the environment variable **or** the input in the transport set-up file (or both) are set TRUE. To avoid any confusion it is not advised to use the environment variable with this version of the PT module.

3 RUNNING THE PARTICLE TRACKING MODULE

The general procedure for particle tracking simulations is:

1. Simulate a transient or steady state ground water velocity field using the MIKE SHE water movement module (WM), menu F.1-F.4. Notice that PT requires the flow results to be stored with the same time interval as the other results in the water movement calculations.

2. Prepare the AD input file (<setupname>.tsf) using the solute transport menu system, menu T.1-T.3. This part covers entering information on initial concentrations, boundary conditions, dispersion coefficients and simulation parameters (time step length and print out times).
3. Prepare the particle tracking input. It is recommended to include the PT input in the bottom of the AD input file (<setupname>.tsf) by using a text editor. So far no menu system has been developed for the specific PT input. Alternatively, a separate file that has to be named <setupname>.ptinp could contain the specific PT input. This file must be located in a subdirectory called *AD*. First, the program will search for PT input at the bottom of the AD input file. If the input is not found a second search for a separate input file will be performed in the AD subdirectory.
4. Run the model from the solute transport menu system, menu T.4.
5. Retrieve model results using the output retrieval program, menu U.9.

4 CREATING INPUT FOR THE PARTICLE TRACKING MODULE

4.1 Recommended Procedure

Input for PT should be included at the bottom of the transport setup file (<setupname>.tsf). In Figure 1 an example of PT input at the bottom of the transport setup file is given.

Important notice: Input is included by editing the transport setup file manually in a text editor. The input should be inserted at the **very end** of the file, i.e. below the "End of File"-line.

A description of the input is given in Figure 1.

```
= = = = = = END OF FILE
PARTICLE TRACKING  : T
PARTICLE MASS      : 10.0
INITSPEC           : -1
LPTBIN             : F
REGZONEFILE        : DIGFILES\regzone.dig
VERTICAL CORRECTION : 1
```

Figure 1 Example of Input at the Bottom of the Transport Set-up File.

- PARTICLE TRACKING: set TRUE enables the particle tracking, set FALSE disables the particle tracking and enables the AD solution.

- PARTICLE MASS: The particle mass is intended for conversion of particle counts (number of particles) to concentration.
- INITSPEC: This number is used to specify how the initialisation of the number of particles for the compartments has to be done. The different possible values that can be used for INITSPEC are listed in Table 1. In case of a positive or zero INITSPEC there will be a constant number of particles all over the domain. In case of a negative INITSPEC the user can distribute the number of particles (INITSPEC=-1) or the concentration (INITSPEC=-2 and -3) by specifying the distribution in T2-files for each layer in the solute transport menu system, menu T.2, see Figure 2. The particles are initially randomly located within the compartment. For option –2 they are only distributed over the saturated part of the compartment. For the other values of INITSPEC they are located anywhere between the bottom and the top of the compartment.
- LPTBIN: set TRUE detailed output to an optional binary file (pt.bin) will be performed. The pt.bin file contains output for all particles at each SZ time step, see Chapter 5 for details. **Important warning:** The binary file can be huge, i.e. maybe more than 1 Gb. Check harddisk space before enabling this option.
- VERTICAL CORRECTION: a new item in this version of PT is correction of the vertical particle coordinate when moving between compartments with changing thickness. This option is by default on and this line can also be omitted. To turn the option of this line should be included and the value should be set to 0.

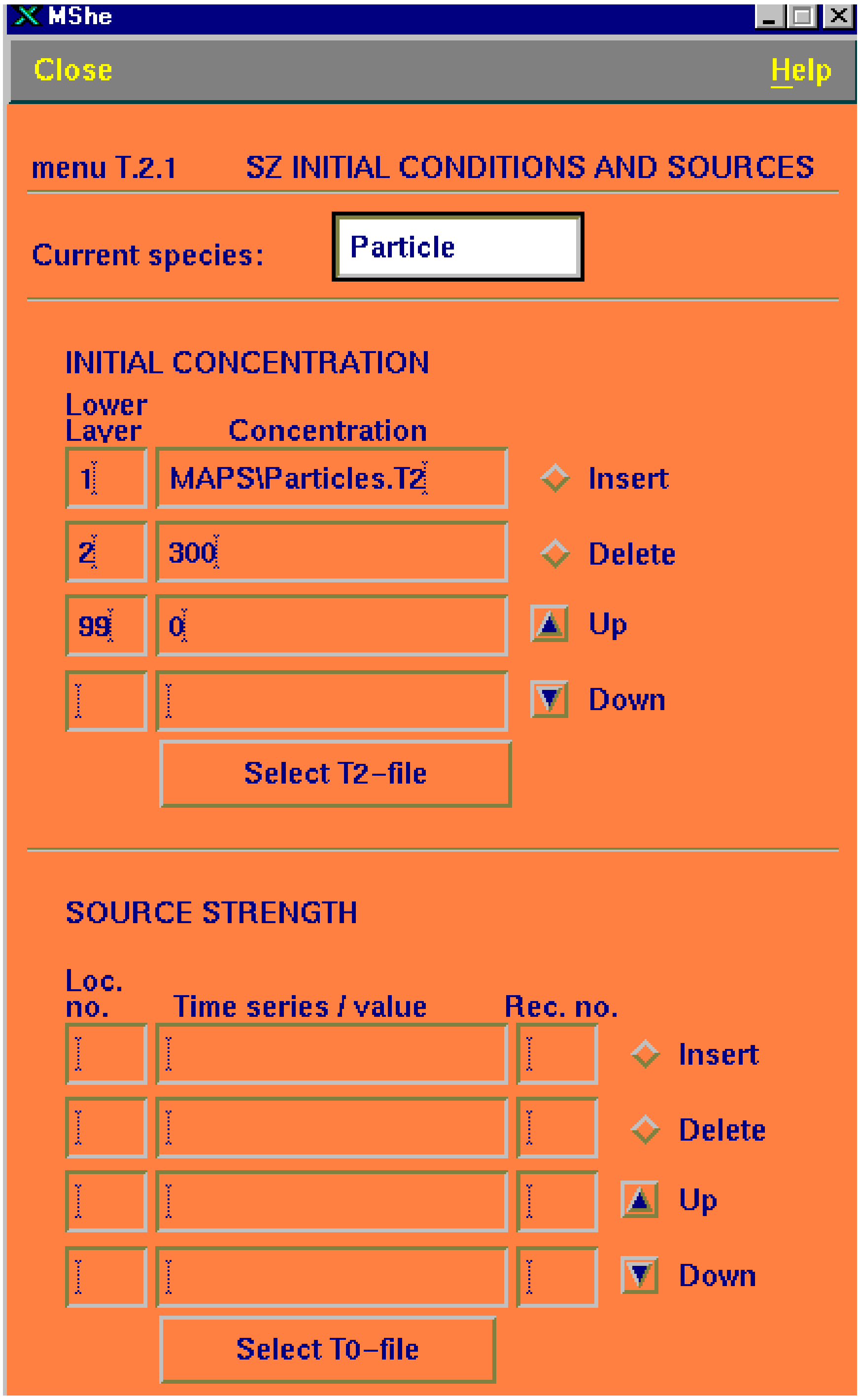

Figure 2 *Example of Specification of the Distribution of Particles for INITSPEC=-1 in T2-files for each Layer in the Solute Transport Menu System, Menu T.2.*

Table 1 Possible Values for INITSPEC

INITSPEC	Meaning
<-3	An error will be generated
-3	An initial particle concentration in the groundwater has to be specified in the AD menu T.2.1. This concentration will be converted to a number of particles by using the particle mass and the saturated volume of each of the compartments. If the resulting number of particles is not an integer a truncation to nearest integer is performed. The particle are distributed randomly over the whole compartment height.
-2	An initial particle concentration in the groundwater has to be specified in the AD menu T.2.1. This concentration will be converted to a number of particles by using the particle mass and the saturated volume of each of the compartments. If the resulting number of particles is not an integer a truncation to nearest integer is performed. The particle are distributed randomly over the saturated part of the compartment.
-1	An initial number of particles in the groundwater has to be specified in the AD menu T.2.1. The particle are distributed randomly over the whole compartment height.
≥0	INITSPEC constitutes the number of particles that will be initially present in each of the compartments of the model domain. The particle are distributed randomly over the whole compartment height.

- REGZONEFILE: The PT module uses the concept of 'registration' cells. This is intended for registering particle data when particles enter certain model compartments. Registration cells can be used to delineate capture zones or to observe particles passing through some region of interest. The information on the registration zones is stored in the regzone.dig file. This is a type 32 type 'dig' file containing polygons or points. The program interpretes the lines in the digfile as:

  a code, x coordinate, y coordinate, layer number.

The first polygon point should have code 1, the last point should have code 3 and the points in between have to have code 2. This is as for a normal type 32 dig file (Appendix A-5 of the Pre- and Postprocessing Module User Guide) with this difference that the fourth field is used for the layer number. An example is shown in Figure 3a. The user can also identify registration cells using single points. The lines have the same appearance as in the type 32 above but the code in field 1 should be 3 for each of the points and each line corresponds to a single point. An example is shown in Figure 3b. **Notice:** if there are no registration cells the name of the regzonefile is omitted from the input.

```
Filetype Datatype Verno: 32  0  540
Textline               : Registration zone code file
UTM XYunit             : 0  2
1    0.0     0.0  1  'Registration zone 1
2 1000.0     0.0  1  'Registration zone 1
2 1000.0  1000.0  1  'Registration zone 1
2    0.0  1000.0  1  'Registration zone 1
3    0.0     0.0  1  'Registration zone 1
```

Figure 3a *Example of Registration Zone Code file using Polygons to delineate Registration Zones. See Appendix A-5 of the Pre- and Post-processing Module User Guide for Explanation of the dig-file.*

```
Filetype Datatype Verno: 32  0  540
Textline               : Registration zone code file
UTM XYunit             : 0  2
3  500.0  500.0 1  'Registration zone cell 1
3  550.0  350.0 1  'Registration zone cell 2
```

Figure 3b *Example of Registration Zone Code File using Points to identify Registration Zones.*

If the user turns on the PT module execution by using the input from the transport set-up file all input for PT will be read from the transport set-up file.

4.2 Alternative Procedure

Alternatively, the PT input can be specified in a separate file named <setupname>.ptinp and located in the AD subdirectory. Please notice that this procedure was kept as an alternative for reasons of backward compatibility and hence not the recommended procedure.

An example of the PT input in this separate file is presented in Figure 4. The input is similar to the input at the bottom of the AD input file except for the input for the registration cells which is not read from a dig file in this case. In the separate file the user has to specify the number of registration compartments as well as the location of each of the registration cell compartments. The location can be specified using row number/ column number from the model grid set-up (option 1) or x/y-co-ordinates (option 2). Please recall that this file was kept as an alternative for reasons of backward compatibility. The text in the file reflects the fact that in previous versions a more restricted form of registration cells called ‘capture’ zones was used. The number of registration cells is therefore called NCAP in this file.

```
INPUT FILE FOR PARTICLE TRACKING MODULE 'particle.inp'

PARTICLE MASS (gram)                                  MASS.......: 10
Number of capture zones/influence zones to estimate   NCAP.......: 1
Number of init. part. in each grid (<0 for conc is used).........: 0
Output to pt.bin (T/F) ..........................................: F

The following lines specifies the location of grid cells for which
data on particles entering the cells is always stored
The two options for specifying these cells.

Option 1:
option   grid-layer grid_column    grid-row

Option 2:
option   grid-layer x-coordinate  y-coordinate

option(1 or 2)   layer           column/x-coord   row/y-coord
---------------------------------------------------------------
1     6     20    20    'regzone1'
```

Figure 4 Example of Input as a separate Input File (AD\<setupname>.ptinp).

Notice: If the user turns on the PT module execution by using the input from the transport set-up file all input for PT will be read from the transport set-up file. This implies that the input from the separate file <setupname>.ptinp is **not** read in this case.

Notice: There is no input for vertical coordinate correction in the old ouput format. The correction will therefore always be active when using the old input format.

5 RETRIEVING, VIEWING AND PLOTTING THE RESULTS

The output of the PT calculations consists of a transport print file (<setupname>.tpf) and a binary transport result file (<setupname>.trf). Optionally, the program can also write output to a binary file called pt.bin.

The output in the transport print file (tpf) is intended for logging program execution. For PT it presents the particle balance during the calculation and some additional information on memory usage.

Results from a particle tracking simulation in the transport result file (trf) can be retrieved by the AD Output Retrieval utility (menu U.9) as maps of different parameters and viewed in the Graphical editor (menu

G.2) as normal T2-data or plotted directly by the Graphical Presentation tool (menu G.1).

For **retrieval** of results follow the specifications for the AD Output Retrieval utility (menu U.9), i.e. select transport result file (*<setupname>.trf*), select output type (*SZ-data*) and select data type (*other data type*). The latter specification is not a usual data type but it is possible to get a list of applicable numbers to be specified for *other data types* by clicking the right mouse button in the edit field:

- 112111: T2-file with the number of particles in each grid cell for the layer
- 112121: T2-file with the average age of the particles in each grid cell for the layer
- 112131: T2-file with the number of registered particles, this is the number of particles that have moved to a compartment which is a registration cell from the compartments in the layer
- 112141: T2-file with the capture zones: This is the registration cell number of the registration cell to which a particle which started from the compartment in the layer has most recently moved to. Notice that the value can change if particles from the cell move through several registration zones and/or not all particles from the cell arrive in the same registration cell.
- 112151: T2-file with the average transport times to the nearest registration cell from each compartment in the layer. If no particles from that cell have entered a registration cell yet thevalue is set to the delete value.
- 112161: Dig-file with the coordinates of current particle locations. Each line contains the values:
    - 3
    - / x-coordinate /
    - / y-coordinate /
    - / z-coordinate /
    - / layer number /
- 11217*i* (with *i* = 1 – 6) Dig-files with the birth locations of particles and the registration cell number of registered particles or the negative value of the sink type code if the particle has been removed from SZ in a cell which is not a registration cell. There is one file for each of the possible sink codes and each layer:
  112171: particle that have reached active cells which are registration zone cells
  112172: particles that have gone to a river sink
  112173: particles that have gone to a drain sink
  112174: particles that have gone to a well sink

112175: particles that have gone to the unsaturated zone
112176: particle that have gone to all other sinks.
Possible codes used for sinks are listed in Table 2. The registration period is from the specified start date in the AD output retrieval menu (menu U.9) until the end of the calculation. Each line contains the values:

- 3
- / birth x-coordinate /
- / birth y-coordinate /
- / registration cell number or negative value of sink-type /
- / travel time (day) /

Notice that data type 112171 can only contain registration cell numbers as the particles in an active cell will only be registered if that cell is a registration cell.

Table 2 Sink Codes for the AD Output Retrieval Data Type 11217i

Value of registration zone	Sink type
-2	River
-3	Drain
-4	Well
-5	Exchange with UZ
-7	Constant concentration cell (boundary)
-13	Constant concentration cell (internal source)

- 11218*i* (with *i* = 1 – 6) Dig-files with the travel times of particles and the registration cell number of registered particles or the negative value of the sink type code if the particle has been removed from SZ in a cell which is not a registration cell. The types are analogues to 11217*i* but with the last two columns switched. There is one file for each of the possible sink codes:
112181: particle that have reached active cells which are registration zone cells
112182: particles that have gone to a river sink
112183: particles that have gone to a drain sink
112184: particles that have gone to a well sink
112185: particles that have gone to the unsaturated zone
112186: particle that have gone to all other sinks.
Each line contains the values:
    - 3
    - / birth x-coordinate /
    - / birth y-coordinate /
    - / travel time (day)/
    - / registration cell number or negative value of sink-type /

In the AD output retrieval menu (menu U.9) the user also has to specify the output date, output file name and output location (only *layer* is important – *ix, iy* and *Qstat no* can be any number).

For **plotting** of results it is recommended to utilise the Graphical Presentation tool and follow the specifications given for this tool:

- Select menu G.1 (Graphical Presentation)
- Select the flow result file (*<setupname>.frf*), which provided the transient or steady state flow field for the particle tracking calculations
- Select grid values
- Click on the *display data types* button. A list of available data types will be displayed including particle tracking results
- Enter the plot number, the data type, the filename, the layer number, and the plot type. The filename is the name of the transport result file (*<setupname>.trf*), which will be located in the folder %sheres%\AD
- Click on the *plot layout* button and specify the *output date*. It is not possible to step through available storage times – use the AD Output Retrieval utility (menu U.9) to determine output times
- Specify all other input parameters as usual and Click on the [*Apply*] button and click on the [*read and plot*] button in the menu G.1.

PT can also store results to a separate binary output file named 'pt.bin' when the LPTBIN option is set true (T). This binary file contains the particle locations at every SZ time step and can be used to calculate detailed flow lines for individual particles. The structure of the pt.bin file is shown in Figure 5. Possible sink type codes used in pt.bin are listed in Table 3. **Notice:** The pt.bin file can be very large and its creation slows down the PT calculation.

```
For each SZ time step:

1 line with
- 4 byte signed integer    : number of particles
- 4 byte signed real       : time of output

followed by 'number of particle' lines with each line containing:
- 4 byte signed integer    : particle ID
- 4 byte signed real       : x-coordinate
- 4 byte signed real       : y-coordinate
- 4 byte signed real       : z-coordinate
- 1 byte signed integer    : particle sink type
```

Figure 5 Structure of the pt.bin File.

Table 3 Possible Sink Codes in the pt.bin File

Sink code	Sink type
0	Unknown
1	Active cell
2	River sink
3	Drain sink
4	Well sink
5	Exchange with UZ (sink)
6	Constant concentration (boundary source)
7	Constant concentration (boundary sink)
9	Zero flux (boundary)
10	Precipitation source
12	Constant concentration cell (internal SZ source)
13	Constant concentration cell (internal SZ sink)

6 PARTICLE TRACKING APPLICATIONS

Using the PT module for delineation of capture zones, for determination of upstream zones, and for groundwater age determination are expected to be among the most popular applications. Thus it has been found useful to explain the procedures for these features in more detail.

6.1 Capture Zones

A capture zone is defined as the area from which the water originates that eventually arrives in a certain point. In terms of the model a capture zone then corresponds to the ensemble of cells containing particles that arrive in certain cell(s). The concept is most often used in relation to wells and then is intended to delineate the area contributing water to a certain well.
The current version of the PT module provides several output data types which can aid at delineating capture zones. A first group of data types is related to the registration cells:

- In the "regzone" file the user specifies coordinates for the cells which are ‘registration cells’.
- During the simulation the particles are moved according to the groundwater velocities and the user specified dispersion coefficients. When a particle enters one of the user specified registration cells; the initial location of the particle (birth location), the current location and the transport time (time of particle birth - current time) are registered.
- This enables the Particle Tracking module to produce the following result types:

   1. **Capture zones (datatype 112141)**
      For each calculation layer a grid map containing numbers, which identify the registration cells to which the most recent particle from the grid cell entered.
   2. **Number of registered particles (datatype 112131)**
      For each calculation layer a grid map defining the number of particles that has reached a registration cell.
   3. **Transport time (datatype 112151)**
      For each calculation layer a grid map defining the transport time to the nearest registration zone cells.

A second group of data types is related to the concept of ‘sink codes’. If the particle is taken out of the model domain it is registered together with a code of the sink that caused the particle to leave the domain.

This allow s the output retrieval to create digfiles containing the following result types:

1. **Birth locations of particles (datatypes 11217*i*; *i* = 1-6)**
   For each calculation layer the birth locations of all particles that have gone to a certain sink. The correspondence between the sink code and the data types is listed in table 4.

Table 4 Possible Datatypes and corresponding Sink Codes

datatype	sinkcode	meaning
112171	*no*	active cell: particles are only registered here if they arrive in an active cell that is at the same time a registration cell.
112172	-2	particles gone to rivers
112173	-3	particles gone to drains
112174	-4	particles gone to wells
112175	-5	particles gone to the unsaturated zone
112176	-7, -13	particles gone to all other sinks

When delineating capture zones for complex flow situations both ‘registration zone codes’ and ‘sink codes’ are needed as particles from the same cell can move to different cells, different sinks within the same cell or move through more than one registration cell. Therefore the output retrieval utility will store the registration cell code instead of the sink code when the cell is a registration cell.

2. **Travel times of particles (datatypes 11218*i*; *i* = 1-6)**
   For each calculation layer the travel times of all particles that have gone to a certain sink. The correspondence between the sink code and the data types is listed in table 5.

Table 5 Possible Datatypes and corresponding Sink Codes

datatype	sinkcode	meaning
112181	*no*	active cell: particles are only registered here if they arrive in an active cell that is at the same time a registration cell.
112182	-2	particles gone to rivers
112183	-3	particles gone to drains
112184	-4	particles gone to wells
112185	-5	particles gone to the unsaturated zone
112186	-7, -13	particles gone to all other sinks

The next chapter highlights the possibilities and caveats of using the module for delineating capture zones for wells which is probably the most common application. After this we will shortly describe a possible alternative use of the capture zone concept in finding ‘upstream zones’

6.1.1 Delineation of capture zones for wells step by step

As pointed out in the previous chapter there are certain limitations to using datatype 211141 to delineate capture zones. A first observation is that particles entering a registration cell containing a well are not necessarily removed by the well. There could be other sinks in the compartment or the well could be a (too) weak sink allowing the particle(s) to slip away to neighbouring cells. So certain cells might appear as belonging to the capture zone while no particles from the cell actually were take out by the well. The opposite is also possible in which compartments which have contributed one or more particles to the compartment containing the well do not appear in the capture zone output. This occurs when not all particles from a certain cell end up in the same cell as the one containing the well of interest. If they instead move to a different registration cell, the compartment from which the particle originated might appear in output data type 211141 as belonging to a different capture zone. It is, in general therefore not recommended to use datatype 211141 for delineating the capture zones for wells but to use datatype 211174 instead. If the model only contains a single well there is also no need for registration cells when delineating capture zones for wells. In general however registration cell information is needed to distinguish the different wells and a registration cell dig-file is needed with one registration code per well(field).

The procedure for delineating the capture zones for wells is then:

a) Edit the Particle Tracking part of the Transport Setup File (*<setupname>.tsf*), see Figure 1.

1. Enable Particle Tracking by setting PARTICLE TRACKING true
2. Specify any positive number for the particle mass (particle mass is not used for delineation of capture zones)
3. Specify the initial number of particles in each grid cell. Initially 2 particles (INITSPEC = 2) in each grid cell is appropriate for many applications. A larger number of particles will result in more accurate results but will slow down calculations. The initial number of particles should also be larger for coarse spatial discretisations in which a small number of compartments is used to represent the model domain.
   Notice: If particles are located in constant concentration cells initially these cells will behave as particle sources so in some applications it might be better to use the INITSPEC = -1 option and specify the particle numbers in the AD menu system (see b.5. below)
4. Specify the registration zones (single cells or areas) in a digfile.
5. Disable the extended print to the binary file by setting LPTBIN false

6. Save the Transport Setup File

b) From the AD menu system do as follows:

1. From menu T.1 select the Flow Result File (*<setupname>.frf*), which will provide the transient or steady state flow field
2. From menu T.1.1 specify porosity
3. From menu T.1.2 specify *no dispersion*
4. From menu T.2 specify species definition name, e.g. Particle. **Notice:** The Particle Tracking module only supports one species
5. From menu T.2.1 specify the initial concentration. If a positive value for INITSPEC is used (see a.3 above) the concentration input in the menu is is not used for delineation of capture zones and any concentration can be used.
6. From menu T.3 specify simulation period. The simulation period should be long (often more than 100 years). One should not worry about taking too long a simulation period: the simulation time is proportional to the number of particles and this number (in the absence of any sources) will decrease with time as the wells remove the particles... .
7. From menu T.3a toggle the *saturated zone* button. Only the saturated zone is supported by the particle tracking module
8. From menu T.3b specify the storage time steps. Storage time step should also be large in accordance with the long simulation period.
9. Save the AD setup
10. Run the MIKE SHE particle tracking (menu T.4)

c) Retrieve datatype 211174 containing the birth locations.

6.1.2 Upstream Zones

Upstream zones can be used to identify the origin of water that passes through a certain area of intrest. Areas of intrest could be the location of an (ecologically) important habitat that is exchanging water with the aquifer that is being studied or a planned drinking water pumping facility. Upstream zones can also be used to delineate the possible locations of pollution sources when pollution has been discovered in a monitoring well. The registration cells are then allocated to the monitoring well locations.
The main difference with the determination of capture zones for wells is that the cells of interest do not (necessarily) contain wells or other sinks and that particles will in general not stop (or be ‘captured’) by the registration cells. If more than one registration cell is used the output for datatypes 112141 and 112171 should therefore be evaluated carefully at different output times as particle could be moving from one registration cell to another and might appear several times in

output type 112171 *i.e.* once for each registration cell the particle has passed through.

6.2 Groundwater Age

The Particle Tracking module includes a facility to estimate the groundwater age. When particles are introduced in the model (e.g. in the precipitation) the "*particle birth day*" is registered along with other information associated to this particle. This enables the model to calculate the average age of the groundwater in each grid cell by calculating the average difference between current time and birth times for all particles located in the cell. Different procedures can be used for estimation of groundwater age. Below one procedure is described where particles are introduced with the infiltrating water originating from precipitation. In this case the groundwater age will represent the transport time from the soil surface to the groundwater storage and thus serve as information of the groundwater storage vulnerability.

6.2.1 Determination of ground water age step by step

a) Edit the Particle Tracking part of the Transport Setup File (*<setupname>.tsf*), see Figure 1.

1) Enable Particle Tracking by setting PARTICLE TRACKING true
2) Specify any positive number for the particle mass (particle mass is not used for determination of groundwater age)
3) Initial number of particles in the groundwater (choose one of the options):

   i) No initial particles will be present in the groundwater by setting INITSPEC=0 (Recommended)
   ii) The initial number of particles in the groundwater will be specified in the AD menu T.2.1 by setting INITSPEC=-1

4) Disable the extended print to the binary file by setting LPTBIN false
5) Finally, no specification of a "regzone" file is necessary (no registration zones are required for the groundwater age determination)
6) Save the Transport Setup File

b) From the AD menu do as follows:

1) From menu T.1 select the Flow Result File (*<setupname>.frf*), which will provide the transient or steady state flow field
2) From menu T.1.1 specify porosity

3) From menu T.1.2 specify the *dispersivities*
4) From menu T.2 specify species definition name, e.g. Particle. **Notice:** The Particle Tracking module only supports one species
5) If option 3) I. was utilised: From menu T.2.1 specify initial concentration for all layers
6) From menu T.3 specify simulation period. The simulation period should be long (often more than 100 years) so that all groundwater compartments have been age determined
7) From menu T.3a toggle the *saturated zone* and the *sources: precipitation/infiltration* buttons
8) From menu T.3b specify the storage time steps. Storage time step should be large to correspond to the long simulation period
9) In the first line in menu T.1.11 specify:

   i) *Location number* = 1
   ii) *Type* = 1
   iii) *Spatial distribution* = 1 (uniformly distributed precipitation source) **or**
   iv) *Spatial distribution* = T2 file (distributed precipitation source)

10) Too many particles will slow down the calculation whereas too few particles will produce an inaccurate result. A trial and error procedure is recommended for determining an appropriate number of particles
11) In the first line of menu T.2.6 specify:

   i) *Location number* = 1
   ii) *Time series / value* = Constant number of particles in the precipitation **or**
   iii) *Time series / value* = T0 file describing the temporal variation of number of particles in the precipitation
   iv) *Record number* = 1

12) Save the AD set-up
13) Run the MIKE SHE particle tracking (menu T.4)

7 TECHNICAL REFERENCE

In the earlier applications of particle models, solute transport problems were solved using particles as an alternative to finite difference or finite element solutions of the advection dispersion equation

$$\frac{\partial c}{\partial t} + \nabla \cdot \left(\underline{u}c\right) - \nabla \cdot \left(\underline{\underline{D}} \cdot \nabla c\right) = 0 \tag{7.1}$$

where c is the solute concentration, t is time, $\underline{u}$ is the ground water pore velocity, and $\underline{\underline{D}}$ is the dispersions tensor. In the particle model a large number of particles are moved individually in a number of time steps according to contributions from advective and dispersive transport. A particle mass is associated to each particle which means that location of a number of particles in a specific volume (here defined by the numerical grid used for the water movement calculations) corresponds to a solute concentration.

For isotropic conditions in the soil matrix the displacement of a particle p is described by the following equation [*Thompson*, 1987]

$$\underline{X}_p\left(t_{n+1}\right) = \underline{X}_p\left(t_n\right) + \left[\underline{u}\left(\underline{X}_{p,n}, t_n\right) + \nabla \cdot \underline{\underline{D}}\left(\underline{X}_{p,n}, t_n\right)\right]\Delta t + \underline{\underline{B}}\left(\underline{X}_{p,n}, t_n\right) \cdot \underline{Z}_{p,n+1}\sqrt{\Delta t} \tag{7.2}$$

where $\underline{X}$ is the particle coordinates, $\Delta t = t_{n+1} - t_n$ is the time step length, $\underline{Z}_{p,n+1}$ is a vector containing three independent random numbers equally distributed in the interval $[-1,+1]$ and

$$\underline{\underline{B}} = \underline{\underline{R}}\,\underline{\underline{B}}^* \tag{7.3}$$

where

$$\underline{\underline{R}} = \begin{bmatrix} \dfrac{u_x}{|\underline{u}|} & \dfrac{-u_y}{\beta} & \dfrac{-\left(u_y^2 + u_z^2 + u_x u_z\right)}{\beta|\underline{u}|} \\ \dfrac{u_y}{|\underline{u}|} & \dfrac{u_x + u_z}{\beta} & \dfrac{u_y\left(u_x - u_z\right)}{\beta|\underline{u}|} \\ \dfrac{u_z}{|\underline{u}|} & \dfrac{-u_y}{\beta} & \dfrac{u_x^2 + u_y^2 + u_x u_z}{\beta|\underline{u}|} \end{bmatrix} \tag{7.4}$$

$$|\underline{u}| = \sqrt{u_x^2 + u_y^2 + u_z^2} \tag{7.5}$$

$$\beta = \sqrt{|\underline{u}|^2 + 2u_x u_z + u_y^2} \tag{7.6}$$

and

$$\underline{\underline{B}}^* = \begin{bmatrix} \sqrt{2\left(\alpha_L |\underline{u}| + D_m\right)} & 0 & 0 \\ 0 & \sqrt{2\left(\alpha_T |\underline{u}| + D_m\right)} & 0 \\ 0 & 0 & \sqrt{2\left(\alpha_T |\underline{u}| + D_m\right)} \end{bmatrix} \tag{7.7}$$

α_L and α_T are the longitudinal and transversal dispersion coefficients, respectively and D_m is the neutral dispersion. Using equation 6.2 repeatedly, the location of a particle at time $t_N = N\Delta t$ can be determined (equation 6.8).

$$\underline{X}_p(t_N) = \underline{X}_p(t_0) + \sum_{n=0}^{N} \left(\left[\underline{u}\left(\underline{X}_{p,n}, t_n\right) + \nabla \cdot \underline{\underline{D}}\left(\underline{X}_{p,n}, t_n\right) \right] \Delta t + \underline{\underline{B}}\left(\underline{X}_{p,n}, t_n\right) \cdot \underline{Z}_{p,n+1} \sqrt{\Delta t} \right) \tag{7.8}$$

After applying equation 7.8 for a large number of particles (N_p) the average solute concentration for an arbitrary volume can be calculated using equation 7.9

$$c_{V,N} = \frac{1}{V} \sum_{p=1}^{N_p} m_p \delta \qquad ; \delta = \begin{cases} 1 & ; \underline{X}_{p,N} \in V \\ 0 & ; \underline{X}_{p,N} \notin V \end{cases} \tag{7.9}$$

where m_p is the particle mass. Using this procedure an accurate solution of the advection- dispersion equation (eq. 7.1) can be obtained [Thompson *et al*., 1987; *Thompson and Dougherty*, 1988; *Kitanidis*, 1994].

The term $\nabla \cdot \underline{\underline{D}}\left(\underline{X}_{p,n}, t_n\right)$ in equations 7.2 and 7.8 is assumed to be much smaller than the remaining term and is omitted for the benefit of the computational speed. This may, however in some situations result in an accumulation of particles near boundaries or stagnation points. [*Kinzelbach and Uffink*, 1989; *Uffink*, 1988; *Kitanidis*, 1994].

Prior to the particle tracking calculations the transient three-dimensional ground water flow field must be obtained using the ground water model (MIKE SHE WM). These velocities are used by the particle model to calculate $\underline{u}\left(\underline{X}_{p,n}, t_n\right)$ using linear interpolation for the spatial interpolation in the three directions in the grid cells. For time integration, simple Eulerian integration is used. The numerical input used by the water movement calculations (MIKE SHE WM [*Abbott et al.*, 1986a, 1986b]) is reused in the particle model as control volumes (see e.g. equation 7.9) and for the specification of initial and boundary conditions. Horizontal movement is only allowed in saturated parts of the SZ model domain. If INITSPEC –2 is used the particles are also moved horizontally in the (fictitious) thin saturated part at the bottom of dry layers. For all other values of INITSPEC there is only vertical movement in the dry layers. The different handling of the INITSPEC –2 option was introduced to allow for a similar behaviour of PT compared to the original finite difference AD solution.

In the current version of PT the vertical position of particles is corrected for changes in compartment thickness when a particle moves horizontally from one compartment to the next. The correction uses the relative vertical location at the old location to determine the new vertical location:

$$z_{new} = \left(\frac{z_{old} - Bottom_{old}}{Top_{old} - Bottom_{old}}\right) \times (Top_{new} - Bottom_{new}) + Bottom_{new}$$

where *old* indicates the previous compartment and *new* the current compartment. The correction is for now only applied when moving horizontally from one compartment to the other *i.e.* there is no interpolation of layer thickness during the movement within a single compartment. This results in sudden changes in the vertical location at compartment boundaries.

In this version of PT the user can use different sinks and sources to respectively remove or add particles in certain model compartments. Possible sinks are:

1) a constant concentration boundary receiving particles
2) a well
3) a river
4) a drain connected to a river or the boundary
5) water movement to the unsaturated zone
6) compartment containing a constant concentration source that is setting the compartment concentration to a lower concentration value than the actual concentration

Possible sources are:

1) a constant concentration boundary from which particles are removed
2) solute concentration of the precipitation
3) a source in the saturated zone with a specified mass rate
4) compartment containing a constant concentration source that is setting the compartment concentration to a higher concentration value than the actual concentration

PT only calculates particle movement in the saturated zone however the volume of water removed by the wells, rivers, drains and the unsaturated zone is known. This volume of water is used to calculate the number of particles that are removed by each of the sinks using the formula:

$$n_i = n \times \frac{V_i}{V_{\text{sink}}} \times \frac{V_{\text{sink}}}{V_{\text{sink}} + V_{tot}} \tag{7.10}$$

with

n_i : number of particles removed to sink i
n : number of particles in the compartment
V_i : volume of water exchanged with sink i
V_{sink} : volume of water exchanged with all sinks
V_{tot} : volume of water in the compartment

Equation 7.10 will calculate the number of particles, which should be removed by the sink at that time step. This is however not necessarily a whole number of particles. PT takes care of this by retaining all the fractions of particles from previous time steps until it can remove a whole particle. Particles are always assigned one by one to the sinks with preference given to the sink in need of most particles. In case there is more than one sink in a cell with each of these sinks requiring the same number of particles there is a random assignment of one particle to one of these sinks. If there are any more particles left after this assignment the next particle will then go to one of the other sinks.

The constant concentration sources and sinks at boundaries or inside the model domain are handled by calculating the particle number that corresponds to the concentration and truncating this value to a whole number. For the mass flux source and the precipitation source the concentration is again converted to a particle number. The whole number obtained by truncating this value is added to the compartment containing the source. The fractions that are left over after truncation are accumulated until a whole number of particles has been attained in one of the next time steps at which time an additional particle is added to the compartment in which the source is located.

Drains can not only appear as sinks that remove particles to rivers or to the boundary out of the model domain. Drains can also transfer particles internally in SZ. If this occurs the particles are moved from one compartment to another by the drain. Notice that there is no time lag in this process.

To enable the model to trace the particles, calculate transport times, capture zones, groundwater age, etc. each particle is associated with a particle identification, model time and location at which the particle was introduced in the model (time and coordinates of ‘birth’). When particles enter sinks or are introduced into the model domain by a source their information is registered together with the source/sink type and the registration time and location before removing or adding the particle. This registration process is also for keeping track of particles that enter registration cells. To avoid repeated registration of particles that have entered a registration cell and which are not (immediately) removed by a sink in the compartment the particle only registers the first time it enters a registration cell.

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