

Modeling the groundwater flow and (lateral) transport

Flow equation

The main features of the groundwater module are:

- The model is a multi-layer model. Each layer is modeled horizontally 2-dimensional in a regularly spaced grid. The coupling between the layers is done using leakage factors.
- The uppermost (first) groundwater aquifer is assumed to be unconfined, the lower aquifers can be confined or unconfined (it is determined by comparing the heads with the upper boundaries of the layers)
- It is possible to use anisotropic conductivities but only in x- and y-direction (without rotated anisotropy). If a rotation is required, the coordinate system should be rotated.
- The connection to surface water is done by leakage approaches within the unsaturated zone model. It is possible to calculate infiltration from rivers as well as exfiltration into the rivers (base flow). If the groundwater reaches the surface of the soil, surface runoff is generated (but in the unsaturated zone model).
- The solution of continuity and flux equations is done using an implicit finite difference approach: Gauss-Seidel-Algorithm with automatic or manual estimation of Successive Over Relaxation Factors (SOR factors). It is scheduled to implement some faster solving algorithms like PCG into the model in later versions.
- The substance transport is done as a big-cell-approach without considering diffusion. It is possible to model the substance transport externally by writing all flux fields to external files.
- spatial distributed parameters for the groundwater model:
 - KX saturated horizontal conductivity (x-direction), 1 grid each aquifer [m/s]
 - KY saturated horizontal conductivity (y-direction), 1 grid each aquifer [m/s]
 - S0 specific storage coefficient (S_0), 1 grid for each aquifer [m^3/m^3]
 - GK leakage factors for layer interaction, 1 grid for each layer [m^{-1}]
 - BQ boundary fluxes (referring to the vertical → recharge), 1 grid for each layer [m/s]
 - BH constant head boundary, 1 grid for each layer [m a.s.l.]
 - AQ aquifer thickness, 1 grid for each layer [m]

Solving the flux equation

The flux equation is get from the continuity equation and from the Darcy-equation. The change of the water storage in a control volume $\partial x \cdot \partial y$ during a time ∂t equals the balance of the inflows into and outflows out of the control volume:

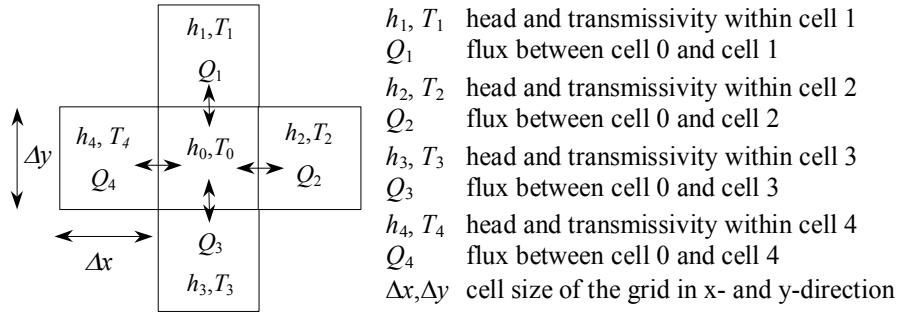
$$\text{div}(T \text{ grad } h) + q + l_{up}(h_{up} - h) + l_{lo}(h_{lo} - h) = S_0 \frac{\partial h}{\partial t} \quad (2.15.1)$$

with	T	transmissivity = aquifer thickness [m] times conductivity K_X (resp. K_Y) [m^2/s]
	h	hydraulic head in the control volume [m]
	q	boundary fluxes perpendicular to the grid cell surface [m/s]
	l_{up}	leakage factor for fluxes between the actual and the upper aquifer [s^{-1}]
	h_{up}	hydraulic head in the upper laying aquifer [m]
	l_{lo}	leakage factor for fluxes between the actual and the lower aquifer [s^{-1}]
	h_{lo}	hydraulic head in the lower laying aquifer [m]
	S_0	specific storage coefficient [1/1]
	t	time [s]

Beside the horizontal fluxes equation (2.15.1) contains also terms for fluxes between aquifers and

the term q , which is introduced to consider extractions or additional inputs by wells or recharge. In case of unconfined conditions in an aquifer below the top aquifer the storage coefficient S_0 of this lower layer is replaced automatically with the storage coefficient from the top layer. This presumes that the other layers use confined values for the storage coefficient whereas for the top aquifer the effective porosity is given as storage coefficient.

To get a discrete equation, a control volume with discrete cell edges Δx and Δy is defined. Also the time is made discrete to Δt . The following equations use local indices between 0 and 4 according to the following scheme.



If in equation (2.15.1) the leakage term is merged together with the perpendicular inflows and outflows (including leakage) through the cells surface to the flux Q_0 and if the divergence of the fluxes is written as balance of the fluxes through the borders of the control volume than a discrete flux equation is given by:

$$\Delta t (Q_1 + Q_2 + Q_3 + Q_4 + Q_0) = [h_0(t + \Delta t) - h_0(t)] S_0 \Delta x \Delta y \quad (2.15.2)$$

with fluxes Q_1 to Q_4 as

$$\begin{aligned} Q_1 &= \Delta x T_{1,0} \frac{h_1(t') - h_0(t')}{\Delta y} & Q_2 &= \Delta y T_{2,0} \frac{h_2(t') - h_0(t')}{\Delta x} \\ Q_3 &= \Delta x T_{3,0} \frac{h_3(t') - h_0(t')}{\Delta y} & Q_4 &= \Delta y T_{4,0} \frac{h_4(t') - h_0(t')}{\Delta x} \end{aligned} \quad (2.15.3)$$

It is assumed that the fluxes during the time step Δt can be represented by the fluxes at the time t' (with $t \leq t' \leq t + \Delta t$) and thus by the heads valid at this time. The transmissivities $T_{1,0}$ to $T_{4,0}$ between the cells 0 and 1, 0 and 2, 0 and 3, and 0 and 4 are averaged as harmonic average of the affected cells:

$$T_{i,0} = 2 \frac{T_i T_0}{T_i + T_0} \quad (2.15.4)$$

with i local indices between 1 and 4

Under confined conditions the local transmissivity in a cell is the product of aquifer thickness and saturated hydraulic conductivity in the matching direction. X- and y-direction may have different conductivities. Under unconfined conditions the local transmissivity is the product of the effective aquifer thickness (only the saturated part of the aquifer) and the saturated hydraulic conductivity in the direction of interest.

The following reformulations presume a regular grid with $\Delta x = \Delta y$ what leads to simplifications of equation (2.15.3). Also the hydraulic heads h' at time t' are expressed by $h(t)$ and $h(t + \Delta t)$:

$$h(t') = (1 - \alpha) \cdot h(t) + \alpha \cdot h(t + \Delta t) \quad (2.15.5)$$

The parameter α has a range of 0 to 1. If α is set to 0 the solution is done explicitly, if α is set 1 the

solution is fully implicit, values between 0 and 1 will cause a partly implicit solution. Explicit solutions are fast because the solution is get in a single step but they tend to numerical instabilities if using long time steps. Implicit solutions can be obtained by using iterative methods or by direct solutions of the linear equation systems. In WaSiM an iterative scheme, the Gauss-Seidel-Algorithm is applied. It is simple and fast enough also for very large model grids, because the time critical part in the model is the unsaturated zone. Usually the model will be applied with time steps of one hour or one day or even longer time steps, thus the use of the fully implicit approach is strongly recommended. If there are oscillations between successive time steps the model gives messages about this in order to allow the user to change some iteration parameters.

If the fluxes from equation (2.15.3) are simplified by $\Delta x/\Delta y = 1.0$ and put into equation (2.15.2) and if the heads $h_0(t')$ are expressed by equation (2.15.5) the head $h_0(t+\Delta t)$ can be expressed by:

$$h_0(t+\Delta t) = \frac{\frac{\Delta x \Delta y}{\Delta t} S_0 \cdot h_0(t) + (F_1 + F_2 + F_3 + F_4) - (1-\alpha) \cdot h_0(t) \cdot (T_{1,0} + T_{2,0} + T_{3,0} + T_{4,0})}{\frac{\Delta x \Delta y}{\Delta t} S_0 + \alpha \cdot (T_{1,0} + T_{2,0} + T_{3,0} + T_{4,0})} \quad (2.15.6)$$

with

$$F_1 = T_{1,0} h_1(t') \quad F_2 = T_{2,0} h_2(t') \quad F_3 = T_{3,0} h_3(t') \quad F_4 = T_{4,0} h_4(t') \quad (2.15.7)$$

Because after a complete step over all grid cells the heads $h_1(t')$ to $h_4(t')$ of the neighboring cells 1 to 4 may have changed, equation (2.15.7) has to be repeatedly processed for the entire grid until the changes between two iteration steps are nowhere greater than a user-specified threshold ε_{max} (of e.g. 10^{-5} m) or until the maximum number of iteration steps n_{iter} has been reached. Both parameters are specified as global parameters in the control file (global means: they are valid for each cell in the grid). To avoid to many iteration steps, for confined conditions the error threshold ε_{max} is automatically increased by a factor 50. This is done in order to consider the much larger effect of very small in- and outflows on the heads compared to unconfined conditions. Thus, a very small flux which is really unimportant for the balance may very well change the heads by e.g. 0.001 m under confined conditions whereas the same flux would change the head under unconfined conditions by e.g. 1e-6 m. Using the Gauss-Seidel iteration scheme it is taken advantage from the fact, that in each iteration step the heads of the cells 1 and 3 (local indices) are already newly calculated values which gives better estimations and thus a faster convergence of the solution.

Acceleration of the convergence of the iteration

In order to minimize the errors of the iteration even faster it is possible to use acceleration factors, the so called successive over relaxation (SOR). Using this method, the differences in the heads between to iteration steps are multiplied by a SOR-factor. This factor can be specified in the control file or it can be estimated automatically during the model run by indicating a negative value for the SOR-factor in the control file. If it is not automatically estimated, the value should be set with care, because too large values will destabilize the iteration scheme. Manually selected SOR-values should be between 1.1 and 1.4. If the model starts to oscillate, this is messaged to the user in order to change also the SOR-factor. In case of an automatic estimation of the SOR-factor the model uses the heads of the actual and the two last iteration steps to calculate an SOR-factor:

$$SOR = 1 + \frac{h(t) - h(t-\Delta t)}{h(t-\Delta t) - h(t-2\Delta t)} \quad (2.15.8)$$

with SOR acceleration factor (successive over relaxation), limited to $1 \leq SOR \leq 2$ [-]

Leakage between aquifers

Fluxes between different aquifers are considered by a leakage-approach. Using Darcy's Law the flux is calculated according to the hydraulic conductivity and the thickness of the assumed clay layer in-between the aquifers. Because usually both variables are unknown they are replaced by a leakage factor l :

$$l = \frac{k'}{d'} \quad (2.15.9)$$

with l leakage-factor [s^{-1}]

k' hydraulic conductivity within the clay layer between the aquifers [$m \cdot s^{-1}$]

d' thickness of the clay layer in-between the aquifers [m]

The leakage fluxes are calculated according to equation (2.15.1) depending on the head difference and the leakage factor. The results are fluxes in m/s perpendicular to the grid cell surface.

boundary conditions

It is possible and required to define grids containing boundary conditions. There are two grids for each aquifer, one containing constant heads and one containing constant fluxes into or out of the cells. The boundary conditions can be set separately for each grid cell but they are valid during the entire model run. For cells with a constant head boundary equation (2.15.6) is skipped. Inputs (positive sign) or extractions (negative sign) are expected in m/s perpendicular to the cell surface. It is also possible to consider lateral boundary fluxes if they are converted considering the grid cell size into matching vertical fluxes. It is not possible to consider temporally variable boundary conditions. Also boundary conditions which are linear combinations of known heads and known fluxes are not explicitly allowed. However, if both grids (constant flux and constant head) have valid entries for a cell, then this is a kind of a combined boundary condition. Such combinations may lead to serious problems with the water balance especially if the hydraulic properties do not match the boundary conditions (too much extraction/inflow and at the same time a fixed head → problems with the balance).

Balance for the 1st aquifer for coupling the unsaturated zone to the groundwater model

The balance of inflows and outflows across the cell boundaries (all six surfaces including ceiling and floor) is converted into an effective rate of change of the groundwater table in terms of water flux. Thus the model of the unsaturated zone gets information about the change of the groundwater table for inclusion into its algorithms. The rate of change of the groundwater table is estimated by:

$$\Delta_{GW} = \frac{h(t - \Delta t) - h(t)}{\Delta t} S_0 \quad (2.15.10)$$

with Δ_{GW} rate of change of the groundwater table in terms of a vertical water flux [$m \cdot s^{-1}$]

$h(t - \Delta t)$ groundwater head in the previous time step [m]

$h(t)$ groundwater head at the end of the actual time step [m]

S_0 specific storage coefficient [-]

Δt time step [s]

Substance transport in the groundwater

The exchange of tracers between unsaturated zone and groundwater and the mixing is considered in the unsaturated zone module. The flux between the last completely unsaturated zone and the groundwater is taken as recharge (or uptake) transporting with it an amount of tracers matching the concentrations of this tracers in the place of the origin of the fluxes. For capillary rise this solute amount is the product of the upwards flow and the concentration of the solute in the groundwater.

Within the groundwater the transport of solutes is estimated using the lateral fluxes and the solute

concentrations in their origin cells. The vertical fluxes are handled in analogy to the horizontal fluxes. After calculating the water fluxes, the corresponding masses of transported tracers are calculated. The balance of mass inflows and outflows with the old tracer content of the cell (all units in 10^3kg or in relative units) is divided by the new water content to get the new tracer concentration:

$$c_0(t+\Delta t) = c_0(t) \cdot \Delta x \cdot \Delta y \cdot n \cdot d + Q_1 \cdot c_{1\cup 0}(t) + Q_2 \cdot c_{2\cup 0}(t) + Q_3 \cdot c_{3\cup 0}(t) + Q_4 \cdot c_{4\cup 0}(t) + Q_{up} \cdot c_{up\cup 0}(t) + Q_{lo} \cdot c_{up\cup 0}(t) + Q_0 \cdot c_0(t) \quad (2.15.11)$$

with	n	porosity [-]
	d	aquifer thickness (confined aquifer) resp. effective aquifer thickness (unconfined aquifer) [m]
	$c_{1\cup 0} \dots c_{4\cup 0}$	tracer concentrations in the four neighboring cells; depending on the flow direction this may be the central cell (index 0) or one of the neighboring cells (indices 1 to 4), units [10^3kg/m^3] or relative concentrations
	$c_{up\cup 0}$	tracer concentrations within the actual or the upper laying aquifer, depending on the flow direction (only if there is an aquifer above, else 0), units like $c_1 \dots c_4$
	$c_{lo\cup 0}$	tracer concentrations within the actual or the lower laying aquifer, depending on the flow direction (only if there is an aquifer below, else 0), units like $c_1 \dots c_4$
	c_0	tracer concentrations in boundary inflows (unimportant for extractions because no concentration changes), units like $c_1 \dots c_4$
	$Q_1 \dots Q_4$	fluxes between the cells 1 ... 4 and the actual cell (index 0) [m^3]
	Q_{up}, Q_{lo}	leakage fluxes, if upper (up) or lower (lo) aquifers are present [m^3]
	Q_0	boundary flux [m^3]

The fluxes Q_1 to Q_4 in equation (2.15.11) are given by:

$$\begin{aligned} Q_1 &= k_{s,1} \frac{h_0 - h_1}{\Delta y} \cdot \Delta x \cdot \Delta t \cdot \frac{d_0 + d_1}{2} \\ Q_2 &= k_{s,2} \frac{h_0 - h_2}{\Delta x} \cdot \Delta y \cdot \Delta t \cdot \frac{d_0 + d_2}{2} \\ Q_3 &= k_{s,3} \frac{h_0 - h_3}{\Delta y} \cdot \Delta x \cdot \Delta t \cdot \frac{d_0 + d_3}{2} \\ Q_4 &= k_{s,4} \frac{h_0 - h_4}{\Delta x} \cdot \Delta y \cdot \Delta t \cdot \frac{d_0 + d_4}{2} \end{aligned} \quad (2.15.12)$$

with	$k_{s,1} \dots k_{s,4}$	saturated lateral hydraulic conductivity in the neighboring cells [m/s]
	$h_0 \dots h_4$	hydraulic heads in the cells 0 to 4 [m]
	$d_0 \dots d_4$	effective thickness of the aquifers in cells 0 to 4

The amount of water within the actual cell which is needed for equation (2.15.11) may be get as balance of the old water content and the inflows and outflows or it may be estimated from the hydraulic head at the end of the time step. If the latter value differs from the first one, the mass fluxes are reduced to the latter one. Thus numerical errors caused by the use of local hydraulic conductivities can be avoided as well as the tracer balance is hold.

balance check when using boundary conditions

When using boundary conditions in the groundwater model, the balance of fluxes and storage changes (which is the basic principle of a groundwater model) will be disturbed. WaSiM deals with boundary conditions in two ways:

- 1) constant head boundaries: the cell is excluded from the Gauss-Seidel-Algorithm because the hydraulic head doesn't have to be calculated for each time step (it is constant...)
- 2) constant flux boundaries: the constant flux is added as additional inflow during the execution of the Gauss-Seidel-Algorithm like leakages from above or below. However, Leakages are implicitly accounted for in the balances, because those amounts of water will internally be transferred from one layer to the other layer. Constant flux boundaries on the other hand, are additional terms which must be accounted in the balance-checksum grid.

In both cases, the initial groundwater table will be taken from the unsaturated zone model. Boundary conditions are then applied on top of this table. Thus, there will be balance differences after the Gauss-Seidel-Algorithm for constant head boundaries (because the fluxes are calculated but the head remains constant) **and** for constant flux boundaries (because the additional flux will lead to an additional change in hydraulic heads which cannot be compensated by the lateral fluxes).

The mass conservation approach of the groundwater model is:

$$\text{div}(T \cdot \text{grad}(h)) + q + l_{up} \cdot (h_{up} - h) + l_{lo} \cdot (h_{lo} - h) = S_0 \frac{\delta h}{\delta t} \quad (2.15.13)$$

where	T	transmissivity = aquifer thickness [m] times conductivity K_X (resp. K_Y) [m^2/s]
	h	hydraulic head in the control volume [m]
	q	boundary fluxes perpendicular to the grid cell surface [m/s]
	l_{up}	leakage factor for fluxes between the actual and the upper aquifer [s^{-1}]
	h_{up}	hydraulic head in the upper laying aquifer [m]
	l_{lo}	leakage factor for fluxes between the actual and the lower aquifer [s^{-1}]
	h_{lo}	hydraulic head in the lower laying aquifer [m]
	S_0	specific storage coefficient [1/1]
	t	time [s]

When solving this equation numerically (see groundwater model description), the values of h are recalculated for each time step. As described above, the boundary conditions will disturb either the left side of the above equation (constant fluxes) or the right side (by keeping the change in storage constant due to constant heads).

The groundwater balance check grid uses these deviations to identify the impact of boundary conditions on the total balance. For each cell, after each time step, the difference between the regular fluxes and the change in storage are calculated and written to a balance-grid:

The above equation in discrete form can be expressed as:

$$\Delta t (Q_1 + Q_2 + Q_3 + Q_4) = [h_0(t + \Delta t) - h_0(t)] S_0 \Delta x \Delta y \quad (2.15.14)$$

For explanation of the entities please refer to the WaSiM description (groundwater model). When the Gauss-Seidel-Algorithm is finished, both sides should be equal, so the term

$$\text{balance} = [h_0(t + \Delta t) - h_0(t)] S_0 \Delta x \Delta y - \Delta t (Q_1 + Q_2 + Q_3 + Q_4) \quad (2.15.15)$$

should be near to 0 (only very small numerical uncertainties will occur). Note: constant flux boundaries are already taken into account by the new h_0 -value whereas the fluxes $Q_0 \dots Q_4$ are calculated based on the heads at the beginning of the interval (without accounting for additional input or output). As can be seen by the above equation, a constant head boundary will cause the left term to be equal to 0 (because $h_0(t + \Delta t) = h_0(t)$), only the sum of fluxes remains. Thus, if the sum of all fluxes is negative (water is flowing out of the cell because constant head is higher than

neighbouring cells' head), the balance will be positive and vice versa.

For constant flux boundaries, on the other hand, the term $[h_0(t+\Delta t) - h_0(t)]S_0\Delta x\Delta y$ will be larger or smaller than the right term $\Delta t(Q_1+Q_2+Q_3+Q_4)$ (because boundary fluxes were added to the head in the Gauss-Seidel-algorithm). Thus, additional inflows (infiltrating water = positive constant flux boundary) will lead to positive balances, additional outflows (pumping = negative constant flux boundary) will lead to a negative balance.

Both boundary conditions could be used in the same model and even in the same cell – their effects on the balance are superposed and written to the balance grid. However: The balance grid will contain the actual value only. To get the total balance for longer time periods, the mechanisms of WaSiM for calculating sum grids must be used.

The setup of the balance grid is simple: The control file must contain a new output grid and a new write grid code, which should be either 13 (sum grid and actual grid will be written at model end) or some other combination of summing up values and writing the last grid (like e.g. 23 for sum grids for every model year).

Example for the extended control file:

```
groundwater_flow]
1                      # 0=ignore the module, 1 = run the module
$time                  # duration of a time step in minutes
1                      # solving method: 1=Gauss-Seidel-iteration
1000                  # max.numberof iterations
0.000001              # max. changes between two iterations
0.0                  # Alpha for estimation of central differences 0.5 =
#                               Crank-Nicholson Method, 0 = fully explicite, 1 =
#                               fully implicite
#-1.20                 # factor for relaxing the iteration if using
$readgrids             # 1=read grids for heads from disk,
2                      # number of layers
25 68                 # coordinates of a control point for all fluxes
$outpath//glog//$grid//.//$year # name of a file containing the flows
# between of the control point
1                      # use Pond Grid
$outpath//$head1grid   # (new) grid for hydraulic heads for layer 1
$Writegrid              # writecode for hydraulic heads for layer 1
$outpath//$flowx1grid   # (new) grid for fluxes in x direction for layer 1
$Writegrid              # writecode for flux-x-grid in layer 1
$outpath//$flowy1grid   # (new) grid for fluxes in y direction for layer 1
$Writegrid              # writecode for flux-y-grid in layer 1
$Outpath//$GWBalance1grid # (new) grid for balance (difference of storage change
# vs. balance of fluxes -> should be 0 or the amount
# of in-/outflows by boundary conditions
13                     # writecode for balance control grid in layer 1 (should
# be at least one sum grid per year --> Code = 20 or 23 (if old grids must be
# read in)
$outpath//$head2grid   # (new) grid for hydraulic heads for layer 2
$Writegrid              # writecode for hydraulic heads for layer 2
$outpath//$flowx2grid   # (new) grid for fluxes in x direction for layer 2
$Writegrid              # writecode for flux-x-grid in layer 2
$outpath//$flowy2grid   # (new) grid for fluxes in y direction for layer 2
$Writegrid              # writecode for flux-y-grid in layer 2
$Outpath//$GWBalance2grid # (new) grid for balance (difference of storage change
# vs. balance of fluxes -> should be 0 or the amount of in-/outflows by boundary
# conditions
13                     # writecode for balance control grid in layer 2 (should
# be at least one sum grid per year --> Code = 20 or 23 (if old grids must be
# read in)
```

The balance grid contains balance values in mm in order to be compatible with all the other grids and statistical output. To calculate a balance over a model run, simply add the average value of this grid to the other balance terms like precipitation, runoff, evaporation, change in soil moisture, change in snow and interception storage change in lake content etc.