Aquifer Physics Modes for Hydrogeological Modeling – an Application of the COMSOL Physics Builder

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Abstract: Although there are porous media and subsurface flow modes available in a toolbox of COMSOL Multiphysics, for hydrogeological modeling some common requirements can not be easily accessed in the graphical user interface. Most crucially, there is no distinction between confined and unconfined situations for permeable layers, i.e. aquifers. Using the Physics Builder for such distinctions *aquifer physics modes* are constructed that enable hydrogeologists to work with COMSOL Multiphysics as they are used to from other specialized software for hydrogeological modeling.

Keywords: COMSOL Physics Builder, Aquifer, Confined Aquifer, Unconfined Aquifer, Hydraulic Potential, Streamfunction

1. Introduction

Aquifers, i.e. permeable layers which are completely or partially saturated with fluid, are the field of expertise for hydrogeologists. There are several important application areas for hydrogeological studies: groundwater flow in general, pumping and injection (for water supply, public, private, industrial, agricultural), contamination and solute transport (risk assessment, remedial actions,…), geothermics and heat transport, geochemistry, and others.

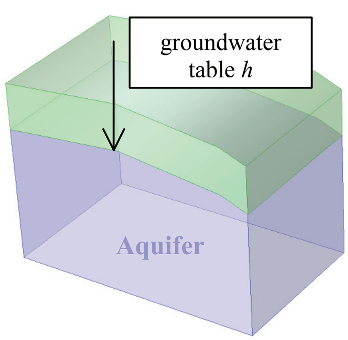

Figure 1. Sketch of an unconfined aquifer

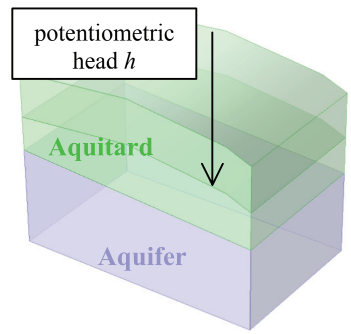

Figure 2. Sketch of a confined aquifer

In hydrogeology there is a distinction between confined or unconfined aquifers, depending on the saturation of the layer. If the layer is saturated up to its top, the situation is confined; if that is not given, the situation is unconfined, also called phreatic. In the latter case the hydraulic head *h* is equal to the groundwater table (Figure 1).

Aquifers are separated by aquitards, i.e. low permeable layers. The uppermost near-surface aquifer is often unconfined. A confined aquifer is confined by an aquitard (Figure 2); hydraulic head *h* is then equal to the potentiometric head. Within an unconfined aquifer the water table separates the saturated zone below from the unsaturated zone above.

Numerical modeling of confined and unconfined aquifers is both based on the common description of fluid flow in porous media. The confined situation can be treated straight forward: the model region is completely saturated. Using Darcy's Law and the principle of mass conservation, leads to the differential equation

$$S_s \frac{\partial h}{\partial t} = \nabla \bullet K \nabla h + Q \tag{1}$$

which is valid in 1D, 2D and 3D situations. Parameters are: specific storage S_s, hydraulic conductivity K and a source/sink-term Q. Equation (1) is to be solved for hydraulic head h as dependent variable. The derivation of equation (1) can be found in classical textbooks on groundwater hydraulics or hydrogeology (Bear 1976, Freeze & Cherry 1979, Fetter 1994), as well as in Holzbecher (2012).

Formulating the equation for the horizontal fluxes (velocity·height) instead of velocities, the differential equation for the confined case in 1D or 2D becomes:

$$S\frac{\partial h}{\partial t} = \nabla \bullet KH\nabla h + q \qquad (2)$$

where H denotes the thickness of the aquifer, which is a constant or a given function in the 1D or 2D model region. The product HK is also known as transmissivity T. S denotes the dimensionless storage parameter and q the source and sink-rate for the entire aquifer.

For the unconfined situation a differential equation is obtained which is only slightly different:

$$S\frac{\partial h}{\partial t} = \nabla \bullet Kh\nabla h + q \qquad (3)$$

As the height of the watertable above the base is variable, the constant H of equation (2) is replaced by the variable h. In contrast to the confined case the coefficient function in the highest order term depends on the unknown variable h, the thickness of the saturated zone. Note that h is measured in relation to the base of the aquifer as zero level (a restriction which is not necessary for the confined case).

Using COMSOL Multiphysics equations (2) and (3) can be modeled in several ways. One can use all modes from the PDE-interfaces and several modes of the classical PDEs. Within the 'Porous Media and Subsurface Flow' toolbox, a modified version of equation (2) can be found. Particularly the storage term is different, as COMSOL Multiphysics works with pressure as dependent variable (instead of head). In addition the 2D version of the COMSOL equation is formulated for a representative layer of unit length through the aquifer. Despite of these differences in storage modelling, here we want to focus on equation (3), which cannot be accessed without tricks using the toolbox.

Using specialized modelling software the hydrogeologist usually has the option to choose between confined or unconfined situations (McDonald & Harbaugh 1988). Depending on the selection either equation (2) or (3) are solved. Here we present two new modes, which enable exactly the same using COMSOL Multiphysics. In order to enable hydrogeological modeling without the need to work with differential equations, *aquifer modes* were developed, which allow to choose confined or unconfined modelling approaches just by mouse-click (Figure 3).

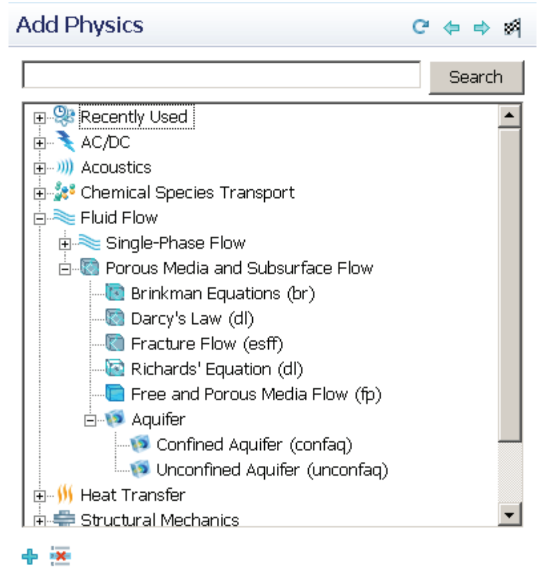

Figure 3. 'Add Physics' options: selection of aquifer modes *confaq* and *unconfaq*

For steady state groundwater flow we will finally describe two more useful modeling options. One mode allows to work without the confined/unconfined choice and lets the program decide, if the situation at a certain location of the aquifer is confined or phreatic. This is based on the hydraulic potential φ that fulfills the Poisson equation

$$\nabla \bullet \nabla \varphi + q = 0 \qquad (4)$$

which is a classical approach (Harr 1962). The relation between the potential φ and hydraulic head h is given by

$$\varphi = \begin{Bmatrix} K \cdot H \cdot h - \tfrac{1}{2} K \cdot H^2 \\ \tfrac{1}{2} K \cdot h^2 \end{Bmatrix} \text{for} \begin{cases} \text{confined} \\ \text{unconfined} \end{cases} \qquad (5)$$

(Holzbecher 2012).

The advantage of the potential formulation is that situations can be handled in which the aquifer is partially unconfined and partially confined.

Another option stems from the utilization of the streamfunction Ψ as dependent variable (Holzbecher 1998). Ψ, for the unconfined aquifer defined by

$$\frac{\partial \Psi}{\partial x} = -h v_y \qquad \frac{\partial \Psi}{\partial y} = h v_x \tag{6}$$

and for the confined aquifer by

$$\frac{\partial \Psi}{\partial x} = -H v_y \qquad \frac{\partial \Psi}{\partial y} = H v_x \tag{7}$$

fulfills the Laplace equation:

$$\nabla \bullet \left({}^{1}\!/_{K} \right) \nabla \Psi = 0 \tag{8}$$

Boundary conditions have to be formulated with respect to the streamfunction, which may be advantageous in some applications. Point sinks and sources cannot be handled with the streamfunction.

2. Physics Builder Implementation

The COMSOL Physics Builder enables the set-up of additional modes, to be used in the same manner as the preinstalled physics modes of COMSOL Multiphysics and its toolboxes. Here we introduce four new modes that can be selected by the user: *unconfaq* and *confaq* for the two situations, described in the introduction. In addition there is the *aq* mode for the potential formulation and the *sf* mode for the streamfunction formulation.

Features determine the way the mode is seen by the user and which options are available. Figure 4 shows the Physics Builder tree and six features that have been implemented for the confined aquifer mode. The other modes are treated analogously.

The first feature (*ConfAqu*) determines the differential equation. Input parameters are K and S. K can be a scalar variable, but for 2D models is allowed to be a matrix also. For the confined aquifer the user has the option to specify transmissivity T alternatively to hydraulic conductivity.

Three additional features provide options for the boundary conditions. The no-flow condition (*Noflow*) is the default. In addition there is the fixed head as Dirichlet boundary condition (*Head*) and the fluid flux as Neumann boundary condition (*Fluidflux*). The Dirichlet condition requires a head value as input, the Neumann condition a velocity value.

There is an additional option on the domain level, by which a source or sink can be specified. This option (*Recharge*) allows the direct input of aquifer recharge in the unit of a velocity.

Moreover there is a feature included to model point sources and sinks (*Pointsource*), which is important for the consideration of wells. This requires the input of a flow rate, either with positive or negative sign, for pumping or injection. Another feature allows the setting of a fixed head at a point (*Pointhead*).

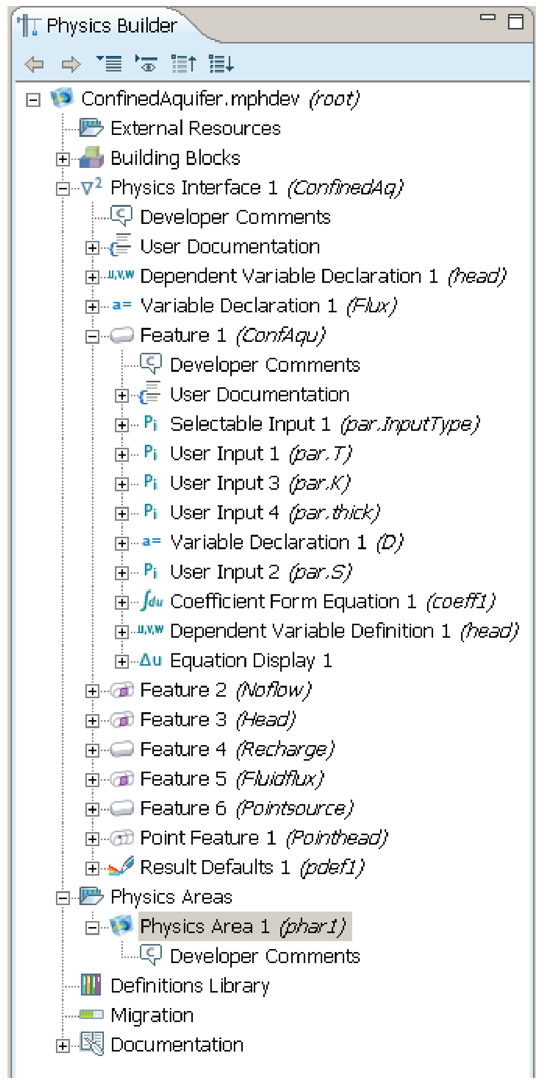

Figure 4. Physics Builder tree for aquifer modes

3. Handling

Allowed dimensions are: 2D, 2D axisymmetric, 1D, 1D axisymmetric. *confaq* and *unconfaq* modes can be steady state or transient, *aq* and *sf* are for steady state only.

In Figure 5 the domain selection box for the confined mode is shown as an example. There is the option to choose between transmissivity input or hydraulic conductivity input (section: Input type). If the hydraulic conductivity option is chosen, the depth of the aquifer has to be specified and the transmissivity is calculated. In the 2D case both K and T can be isotropic, diagonal or anisotropic. In the latter cases all matrix values can be entered manually. The storage parameter is relevant in transient models.

In the unconfined mode only conductivity and aquifer thickness have to be entered. In the streamfunction and aquifer mode only the isotropic situation can be modelled.

Concerning boundary conditions, fixed head and flux conditions can be handled in the *unconfaq*, the *confaq* and the *aq* mode. The first are Dirichlet type, the latter Neumann type conditions. In the *sf* mode the Dirichlet condition concerns streamfunction. A constant value thus represents a streamline. In the *sf* mode Neumann conditions represent tangential fluxes. Thus the condition $\partial\Psi/\partial n = 0$ stands for normal flow across the boundary. Cauchy type boundary conditions are not yet implemented.

In the aquifer modes point conditions can be specified for head values. Moreover pumping and infiltration wells can be introduced easily by point conditions, too. In *sf* mode there is a point condition for streamfunction.

4. Verification and Applications

For the verification of the new modes we choose the flow pattern towards a well in a 1D regional flow field as a benchmark example. We demonstrate the performance of the aquifer mode and of the finite element approach for the hydraulic head in the vicinity of a well. As parameters we choose hydraulic conductivity K=10^{-3} m/s, aquifer thickness of 1 m, and pumping rate Q=10^{-3} m^3/s. The well is located at the origin of a square and we use no-flow boundary conditions at boundaries with constant y-value (in figure: top and bottom), and head condition h_0=0 at constant x-boundaries (left and right).

Using the *confaq*-mode a parametric sweep is performed, for the length of the model region, shown in the legend of Figure 6 (in [m]).

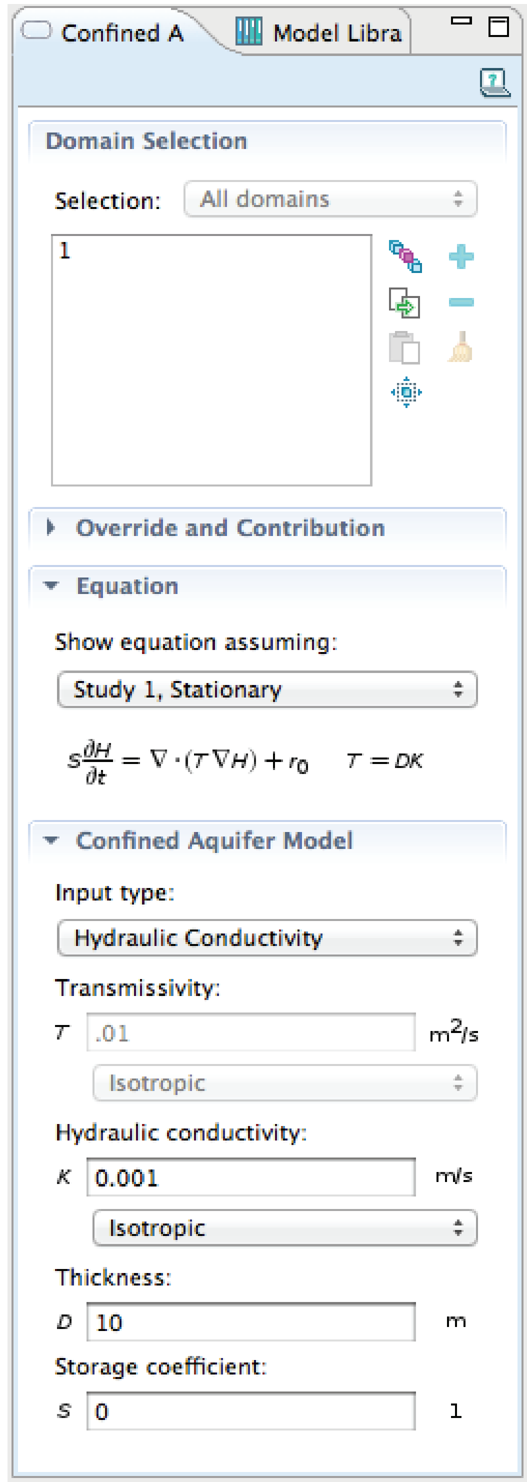

Figure 5. Domain selection input for the confined aquifer mode (*confaq*)

For intercomparison, the analytical solution, derived for the infinite model region, is depicted in the figure additionally. The formula for the analytical solution for hydraulic head is:

$$h(x) = h_{init}(x) + \frac{Q}{2\pi T}\log(x) \qquad (9)$$

(see for example: Holzbecher 2012), where h_{init} denotes the initial head distribution before pumping. As reference point for the analytical solutions we choose the position $(x_{ref},y_{ref})=(0,1)$.

With increasing model extension the convergence of the potentiometric head of the numerical solutions towards the analytical solution can be observed clearly. With increasing model length the influence from the boundary conditions, which are different in numerical and analytical solutions, becomes less relevant (as the boundaries are further away).

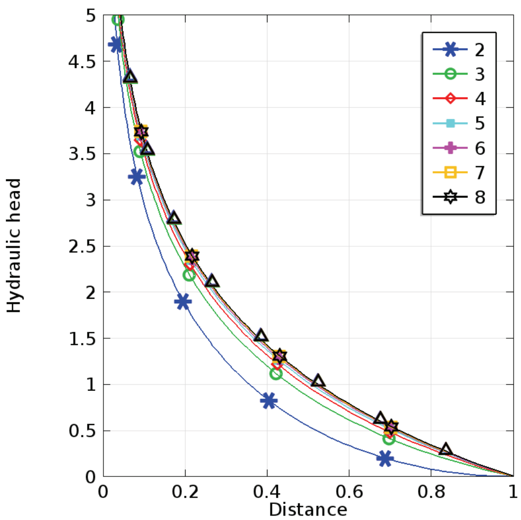

Figure 6. Hydraulic head in the vicinity of a pumping well for the confined aquifer; numerical solutions for different model lengths, according to legend; analytical solution indicated by black triangles; all units in [m]

Figure 7 depicts the solution in the 2D plane for an unconfined situation with baseflow and well. The default output, defined in the Physics Builder, provides a surface plot of hydraulic head and a flownet consisting of streamlines and head contours (isopleths). The regional baseflow is from left to right, i.e. the red colour represents high head values and blue colour low values.

We extend the examination of the just described pumping benchmark, comparing head distributions for the confined and for the unconfined situation, and for the case, in which the aquifer is partially confined and partially unconfined. For the simulations we use the *confaq*, the *unconfaq* and the *aq*-mode.

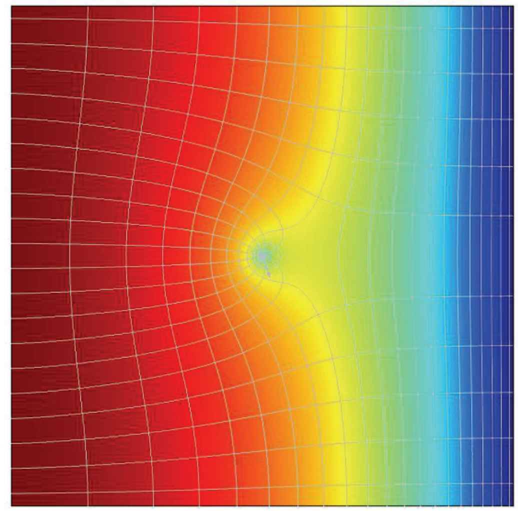

Figure 7. Flow towards a well in an unconfined aquifer; flownet consisting of streamlines and isopleths; an *unconfaq* mode application

In all three cases the same fixed head Dirichlet boundary conditions are prescribed at the upstream and downstream boundaries at a distance of 10 m from the well. The aquifer thickness is 1.5 m.

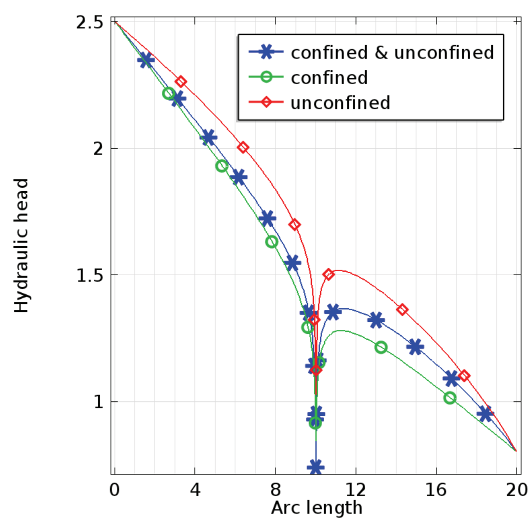

Figure 8. Hydraulic head around a pumping well for the confined, unconfined and partially confined/unconfined cases; numerical solutions with *aq*-, *confaq*- and *unconfaq*-modes; all units in [m]

Figure 8 depicts head distributions along the symmetry axis (horizontal center line in Figure 7). Obviously there are recognizable differences. For a real situation, in which the aquifer is confined in parts and unconfined in the remaining, models with predefined confined or unconfined state for the entire model region, deliver erroneous results. The computation for the confined case leads to an overestimation of head values, while the assumption of unconfined state leads to an underestimation.

The *aq*-mode enables the modeling of flow situations, in which there is a change from confined to unconfined state. The model itself determines the aquifer state (confined or unconfined). This has the advantage that the user does not have to know about the confined/ unconfined situation in the aquifer beforehand.

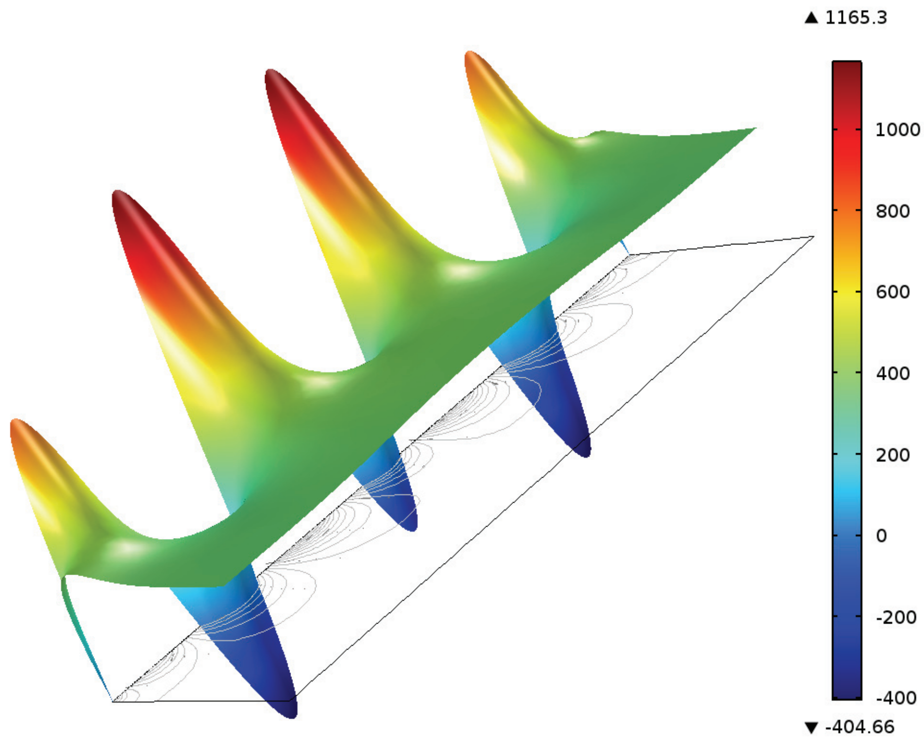

Figure 9. A drainage basin model as streamfunction (*sf*) mode application

As final example Figure 9 we demonstrate an application of the streamfunction mode. Here the flow in a vertical cross-section through a drainage basin is considered. Due to local infiltration processes at the surface here an idealized double-sinusodial head and flow pattern is prescribed. The model approach goes back to early numerical studies of Tóth (1962, 1963). Jiang *et al.* (2011) give an analytical solution for these conditions. In our model we utilized a Dirichlet boundary condition for streamfunction at the upper model boundary

$$\Psi(x) = \Psi_1 \sin\left(\frac{\pi L}{x}\right) + \frac{\Psi_2}{m}\sin\left(\frac{\pi L}{mx}\right) \quad (10)$$

with constants Ψ_1 and Ψ_2 (Jiang et al. 2012). Here we choose m=7, $\Psi_1 = 500$, $\Psi_2 = 5000$ and L=7000 m.

Figure 9 shows the output for the streamfunction as a surface above the model region plane. On the plane streamlines are visualized as contour lines of the streamfunction (grey lines).

This representation has the nice property that a flow pattern results in which all flow tubes have the same flow rate. Thus the density of streamlines at a certain position is a direct measure of the local flow velocity (such topics were discussed by: Holzbecher & Sauter 2010). For that property the equidistant levels of the streamfunction have to be selected.

Using the streamfunction mode the boundary conditions have to be defined in a different way. For example total fluxes can be specified at open boundaries, leaving the local velocity distribution along the edge open to the model.

5. Summary & Discussion

In hydrogeological studies and hydrological studies of the subsurface, saturated and partially saturated layers, so called aquifers, are mostly not resolved in the vertical direction. The spatial dimension of the problem for a single aquifer is thus reduced by 1: 2D instead of 3D, and 1D instead of 2D in vertical cross-sections. This simplification is in fact mostly referred to and discussed as *Dupuit assumption* (Fetter 1994).

For numerical modeling the reduced model complexity due to the lower space dimension usually is of considerable advantage: less computer resources, execution time and storage, are needed. Moreover, usually the understanding of a model is improved, if the relevant phenomena can be captured in reduced spatial dimensions.

The introduction of such an approach in COMSOL Multiphysics, even using the subsurface toolbox, is not straightforward. Formulation of the storage term is quite different. It is particularly complicated to cope with the different cases of a saturated or of an only partially saturated (confined and unconfined) situation.

For that reason we use the Physics Builder, included in COMSOL Multiphysics, to set up new physics modes for confined and unconfined aquifers: *confaq* and *unconfaq*. With these the user with hydrogeological background can set up models in a familiar way using established parameters and variables.

For the steady state we construct another new mode (*aq*), which allows aquifer modeling without fixing confined or unconfined conditions for the entire model region. That is done by the model itself and thus enables to cope with situations in which the aquifer type may change spatially.

Finally, the *sf*-mode utilizing the streamfunction approach enables the construction of exact flownets with equal fluxes within flow tubes between adjacent streamlines.

Geometries with different layers of aquifers and aquitards can be handled easily using the new modes. The heads in adjacent aquifers can be treated by linear extrusions. In that way separating aquitards, in which due to their small conductivity the flux is almost vertical, can be included easily.

The new modes should not be utilized, if there is flow of significant size in the vertical direction within the aquifer, i.e. in which the Dupuit assumption is not valid. For example: for situations, in which pumping or injection take place at different depths in the same aquifer (for an example see: Jin *et al*. 2012) the aquifer modes are not applicable. However, in the majority of groundwater model applications it is justified to neglect vertical fluxes.

The COMSOL Physics Builder is a powerful tool, by which new physics modes can be constructed for specialized applications, which are not considered in the COMSOL Multiphysics mode list. Using the *Physics Builder Manager* the modes can be compiled into an archive, which then can be distributed for use by interested modelers in the specialized application field. I hope that the here described modes find interest among hydrogeologists, who in that way can profit not only from the described special properties of the modes, but also from all the advanced features of COMSOL Multiphysics finite element software.

For the availability of the aquifers modes, see website: ***www.geo-sol.de***.

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