

The Use of COMSOL Multiphysics in Teaching Groundwater Flow and Transport*

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For teaching groundwater flow and transport we currently apply COMSOL Multiphysics software. We have two main goals. At first, to familiarise course participants with the basic concepts and phenomena of the subject. Second, to enable students to handle a modelling tool in general. We describe the fundamentals and give examples of exercises that include several features of the modelling options. The multiphysics concept, on which the software is built, is best suited for the modelling of hydrogeological systems, in which flow and transport are connected or even coupled. The user-friendly design of COMSOL makes the software well-suited for use in the class-room for both the above-mentioned purposes. The students benefit from the easy handling of model input, which is completely performed within the graphical user interface. Most striking are the post-processing options for numerical and graphical output.

Keywords: groundwater flow and transport; saltwater intrusion

INTRODUCTION

IN THE PAST DECADES groundwater modelling has become an important tool in both research and practical work, which has also triggered increased interest in modelling courses at universities. From a methodological point of view groundwater modelling can be subdivided into flow and transport modelling. Flow modelling deals with the movement of water, whereas transport modelling is concerned with the distribution and migration of solutes or heat in the subsurface.

Flow modelling is relevant for the management of water supply systems and supervision of hydraulic works. Transport modelling is mainly applied to problems in which groundwater quality is of concern. Advanced features of groundwater modelling are reactive transport modelling and the consideration of density-driven flow due to changes of salinity and/or temperature.

A two-part course in alternate semesters (Modelling I and II) at Freie Universität Berlin deals with fundamentals of flow, such as Darcy's Law, and reactive transport, such as Fick's Law coupled with kinetic laws. The course addresses students with little or no modelling experience and skills. Here we present the course concept as well as our experiences. There are two main goals. The first goal is to familiarise students with the basic concepts and phenomena of the subject. For that purpose, simple

models are set up and examined by the students, hands-on the computer. The groundwater flow course is mainly concerned with the altered flow regime in an aquifer due to the installation of landfills or other waste disposal facilities or of wells. The transport course deals with the simulation of the processes governing the spatial and temporal distribution of contaminants in an aquifer. Processes such as advection, diffusion, dispersion, sorption, reaction, as well as decay and degradation are studied separately or in combination. Here the term 'transport' is used in a general sense, including processes like sorption and degradation, as they are most important in environmental studies concerned with groundwater quality.

The second goal is to enable students to handle a modelling tool in general. Here, the mathematical concept of a model region with realistic boundary and initial conditions described by solutions of partial differential equations is introduced and outlined. Under classroom supervision application examples are set up by the students, starting from relatively simple groundwater flow patterns under different boundary conditions to combined flow and transport simulations, steady and transient, extended also for density-driven flow problems such as saltwater intrusion.

The COMSOL Multiphysics software is currently used for the course at Freie Universität Berlin. We chose COMSOL Multiphysics because it (i) provides an efficient tool to handle the different modelling tasks, involving flow and

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transport, numerically and (ii) enables students to gain a deeper understanding of these complex topics owing to its flexible interface for pre- and postprocessing.

In the course we mainly use the Earth Science Module (ESM), an additional COMSOL toolbox for COMSOL Multiphysics, especially designed for geo-sciences and -engineering. We pick out those few ‘physics’ modes that address groundwater modellers directly. However, these few modes are sufficient for dealing with most problems in aquifers, concerning water quantity as well as water quality.

In COMSOL-ESM it is also possible to simulate unsaturated flow (using Richard’s equation), which is especially relevant for soil scientists and in studies concerning near-surface problems and phenomena. Correspondingly, solute transport can also be treated in variably saturated environments such like soils or sediments of ephemeral streams or reservoirs. These topics are not part of the groundwater course, in which we solely deal with the water saturated situation. Heat transport in the subsurface can also be treated using COMSOL Multiphysics, as well in the base module as in the ESM toolbox. This option and the corresponding modes are mentioned in the course, but examples within the course deal with mass transport only. The participants who manage mass transport models during the course will surely have no problems coping with heat transport either.

GROUNDWATER FLOW MODELLING

Fundamentals

As COMSOL Multiphysics is a program for the solution of partial differential equations, a short introduction to these equations is necessary, although a detailed understanding of differential equations is not a major concern of the course. The relevant differential equation, implemented in the COMSOL Earth Science Module (ESM), is the following [1, 2]:

$$\nabla \left(\frac{K}{\rho g} \nabla (p + \rho g z) \right) = Q \quad (1)$$

The application mode is reached under ‘Earth Science Module -> Fluid Flow -> Darcy’s Law’, and is internally named ‘esdl’ (Earth Science Darcy’s Law). Dependent variable is the pressure p . Equation (1) is a differential equation in 1D, 2D or 3D. K denotes hydraulic conductivity (physical unit [m/s]), ρ fluid density, g the constant of gravity, and z the coordinate in vertical direction. Q is a general source- and sink-term with the physical unit [1/s]. Using COMSOL, scaling terms not shown in equation can be considered additionally.

An alternative formulation offered by COMSOL ESM is given using permeability κ (physical unit [m²]) instead of conductivity:

$$\nabla \left(\frac{\kappa}{\eta} \nabla (p + \rho g z) \right) = Q \quad (2)$$

where η denotes fluid viscosity.

An important variable for geo-engineers, which appears in both formulations (1) and (2), is hydraulic head h , defined by:

$$h = \frac{p}{\rho g} + z \quad (3)$$

In terms of h the differential equation (1) can also be re-written in the compact form:

$$\nabla (K \nabla h) = Q \quad (4)$$

which is a familiar formulation for most groundwater experts. Equations (1) and (4) are not exactly equivalent because the density appears differently in the inner differential operation. The difference may be relevant only for variable density fluids, which are discussed in the ‘Coupled flow and transport’ section below.

A special case is given for 1D and 2D models in a horizontal cross-section, for which the differential equation transforms to the formulation:

$$\nabla (KH \nabla h) = \tilde{Q} \quad (5)$$

with variable aquifer depth H . Note that the source term \tilde{Q} has the unit [m/s].

Hydrogeologists distinguish between confined and unconfined aquifers. For the confined aquifer the coefficient KH is equal to the transmissivity T , with physical unit [m²/s]. For unconfined aquifers the height is variable. The formula $H = h$ holds if the zero level for piezometric head coincides with the base of the aquifer. Unfortunately the distinction between confined and unconfined aquifers is not yet reflected in the COMSOL ESM. However, the user can easily circumvent this problem. For the unconfined aquifer we chose to use the scaling coefficient for flux to consider the effect of the changing aquifer depth. The students have to enter the COMSOL variable ‘H_esdl’ as scaling coefficient. ‘H_esdl’ is the default name for the hydraulic head h given internally in COMSOL ESM. For their first exercises we recommend the students not to change default names.

All major types of boundary conditions are predefined in COMSOL ESM. The user may choose between five different types: inward flux (1), atmosphere or gauge (2), zero flux/symmetry (3), mixed (4) and hydraulic head (5). In almost all hydrogeological models there is a fixed head to be specified at least at some parts of the boundaries, which is accomplished by using type (5). Equally important is the zero flux condition, which is valid at the interface to impermeable strata, but also at water divides and, more generally, along streamlines. In all these cases condition (3) has to be chosen. When the flux is known, the value for the corresponding velocity can be entered using option

(1). In condition (2) a zero pressure level is implicitly specified, as it is characteristic for boundaries connected with the atmosphere. With condition (4) more complex situations can be considered in which a head or pressure value is connected with a flux or velocity term. Near ephemeral water-bodies such a connection needs to be taken into account.

Exercise

As an exercise in which several of these conditions and typical settings of parameters appear, the students treat an example that was originally proposed during the international HYDROCOIN workshop, where it was classified as level 1, case 7 [3].

In the example, groundwater flow is to be modelled around a hypothetical shallow land-disposal facility for low and intermediate level radioactive waste in argillaceous media. The waste is envisaged as being disposed of in parallel trenches about ten metres below the earth's surface, allowing a 2D model approach for a representative cross-section. A cross-section showing four trenches is depicted in Fig. 1. The cross-section has two types of trenches: slender ones with a width of 25 m and a height of 1 m, and a second type with a width of 20 m and a height of 5 m. The trenches are filled with concrete-encapsulated waste and covered with rolled clay. The idealised situation, shown in Fig. 1, is specified in the test-case definition, representing a system of various geological strata between an impermeable base at the bottom and a sloping groundwater table at the top. The total length of the cross-section is 200 m and the maximum height is 25 m.

The site consists of horizontally bedded clay, resting conformably on a 3 m thick aquifer. In the model the porous medium is isotropic, but properties, hydraulic conductivities and porosities vary with depth. It is assumed that the logarithms of hydraulic conductivity and porosity vary linearly for depths between the values given. The user has to utilise functions for the input of these dependencies. For the easy input of such functions, the

COMSOL graphical user interface offers a special functionality under 'Options -> Functions'.

The HYDROCOIN project considers two scenarios for the waste trenches. In one scenario it is assumed that the cement remains intact and has a constant low conductivity of $K = 10^{-10}$ m/s. In the other scenario the poor quality concrete is degraded by various physical, chemical and biological processes and thus retains a high conductivity of $K = 10^{-6}$ m/s. The boundary conditions for the model reflect the superposition of two regimes. There is a hydraulic gradient in a horizontal direction: hydraulic head h decreases from a prescribed value of 25 m at the left boundary of the cross-section. The second regime acts in a vertical direction and is mainly induced by the condition that there is outflow to the atmosphere at the right side of the model region. Thus boundary conditions of types (2), (3) and (5), as noted above, have to be applied.

The HYDROCOIN test case requires trajectories as output, starting from 12 specified locations. For visualisation of the model output we request from the students:

- surface plot
- contour lines for head contours
- arrows
- streamlines

the latter two based on the COMSOL ESM variables 'u_esdl' and 'v_esdl', which are the predefined names for the components of the velocity vector in the 'esdl' mode. An exemplary output is depicted in Fig. 2.

In addition, we want the students to compare the outcome of the two scenarios, one with an increased hydraulic conductivity and one with a reduced conductivity in the waste blocks. It is easy to realise that in the first case the streamlines gather in the waste blocks, whereas the blocks resemble an obstacle in the latter case. Isopotential lines, produced in post-processing mode, reflect such different behaviour.

In the last part of the course dealing with flow, we introduce the modelling of wells, a very impor-

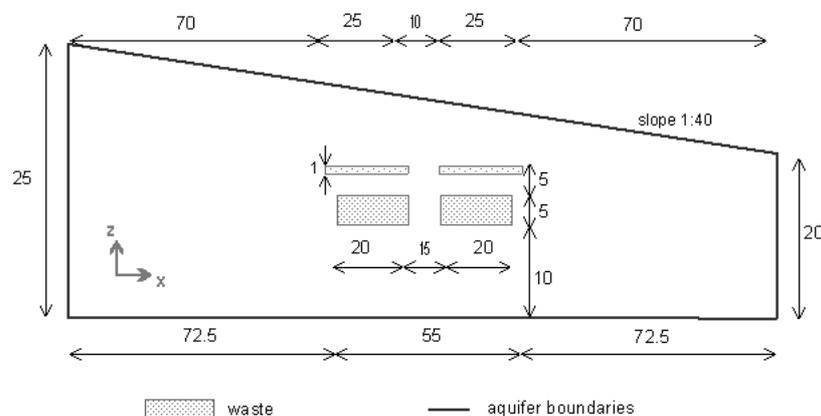


Fig. 1. Set-up for the HYDROCOIN level 1, case 7 exercise model.

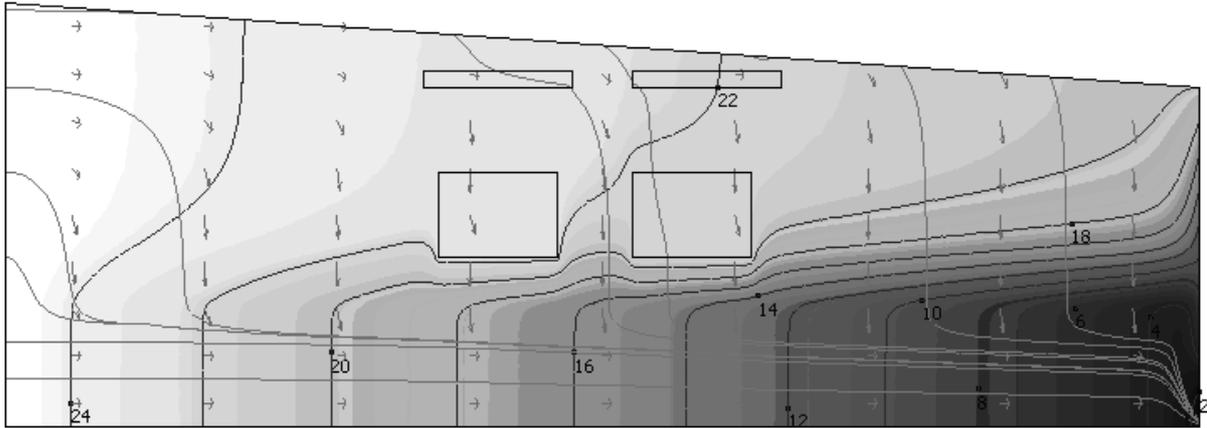


Fig. 2. Exemplary student result for the HYDROCOIN level 1, case 7 exercise model (see Figure 1); surface and contour plots of hydraulic head distribution, velocity field, represented by arrows, and streamlines.

tant feature for geo-engineers. Wells can be introduced easily using the COMSOL ESM. Well positions can be set in the 'Draw mode'. The pumping rate is specified under 'Physics -> Subdomain Settings -> Point Settings -> Flux'. Default physical unit is [m²/s]. In this paper we skip a more detailed description of the corresponding exercise.

MASS TRANSPORT MODELLING

Advection and Dispersion

Transport in general, not only in groundwater, includes the processes of advection, i.e. the shift with the flow field, and dispersion. Dispersion is a general term for mixing processes; it includes molecular diffusion at the smallest scale and mixing due to 'inhomogeneities' of the flow field. The latter is caused by different processes at various length and time scales [1, 2]. The transport equation:

$$\frac{\partial}{\partial t}(\theta c) = \nabla \cdot (\mathbf{D} \nabla c - \mathbf{v} c) \quad (6)$$

is a differential equation for the unknown concentration c , with porosity θ , dispersion tensor \mathbf{D} and velocity vector \mathbf{v} as parameters. Note that \mathbf{v} denotes the Darcy velocity, also called filtration velocity or seepage velocity. \mathbf{D} is the dispersion tensor, defined by:

$$\mathbf{D} = (D_{ij}) = \left((\tau D_m + \alpha_L v) \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{v} \right) \quad (7)$$

with longitudinal dispersivity α_L , transversal dispersivity α_T , tortuosity factor τ and molecular diffusivity D_m . The subscripts i and j denote indices related to the directions of the coordinate system and δ_{ij} is the Kronecker symbol.

In the COMSOL software a transport simulation can be reached under 'Convection and Diffusion' mode. Then, special settings connected with

the interaction of the porous medium (such as porosity and tortuosity) have to be entered 'manually'. For the geo-engineer it is more convenient to utilise COMSOL ESM, where the transport equation is reached under 'Earth Science Module -> Solute transport -> Saturated Porous Media' and named 'esst' (Earth Science Solute Transport).

All relevant boundary conditions are also included in COMSOL ESM. There are six options: concentration (1), flux (2), no flux/symmetry (3), advective flux (4), dispersive flux (5) and general Neumann expression (6). Most important are the conditions (1), (3) and (4). (5) is a generalised version of (4), and (6) is a generalised version of (5). These are examined by the students in simple model set-ups.

In the course the basic features of transport are explored for the simple 1D situation of a column experiment. A fluid, containing a tracer substance, enters at a constant rate from one side into a system that does not contain the substance initially. In most exercises we use an inflow concentration of 1 and an initial concentration of 0.

At the inlet we use the boundary condition of type (1) with a specified concentration, being different from the initial condition. At the outlet we use condition (3), for which conditions (4) or (5) (with appropriate parameters) can be used alternatively.

The analytical solution for such a 1D situation is given by:

$$c(x, t) = \frac{c_{in}}{2} \left(\operatorname{erfc} \left(\frac{x - vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{v}{D} x \right) \operatorname{erfc} \left(\frac{x + vt}{2\sqrt{Dt}} \right) \right) \quad (8)$$

according to Ogata & Banks [4], which can be easily implemented by the students by using COMSOL expressions. The mathematical functions 'exp' and 'erfc' are available in COMSOL.

In Fig. 3 we compare the numerical solution obtained by COMSOL with the analytical solution of Ogata-Banks. For demonstration purposes we

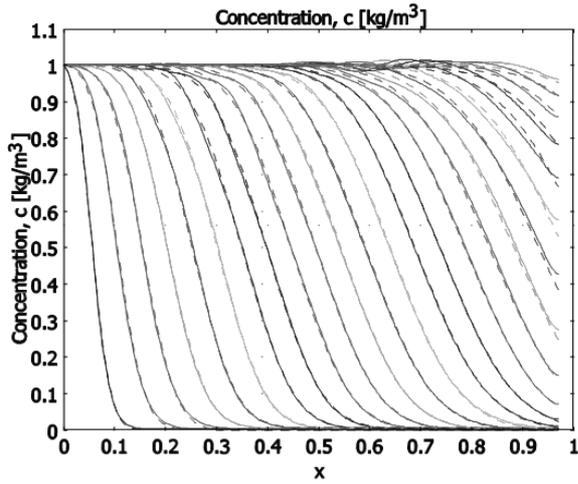


Fig. 3. Comparison of numerical (solid lines) and analytical solutions (broken lines) for an advancing front problem, described by the 1D convection-diffusion equation.

choose an advection-dominant set-up that is relatively difficult to simulate ($D = 0.01 \text{ m}^2/\text{s}$, $v = 1 \text{ m/s}$). We take a relatively coarse mesh (121 elements) and require a relative and absolute tolerance of only 1/100. The figure shows concentration profiles along the length of 1 m with time steps of 0.05 s. The numerical solution is given as a solid line, the analytical Ogata-Banks solution as a broken line.

The first numerical results, as shown in Fig. 3, are poor. There are oscillations near the maximal concentration line, which increase with simulation time. The students examine various possibilities to avoid these un-physical oscillations. One option is to refine the mesh in the ‘mesh mode’. Another option is to reduce the accuracy parameter for the solver. Additionally there are options to suppress artificial diffusion, for which COMSOL has a special input box available for all transport modes.

The exercise makes clear that mesh refinement and solver accuracy are important ‘switches’ to improve the numerical solution. Such a demonstration is especially crucial for those students who have never dealt with models before, as this is the first time they encounter numerical parameters. We teach them to check the final version of every model by grid refinement, if possible. However, it is important for the students to note that, while oscillations are successfully suppressed, the deviations between analytical and numerical solutions at the outlet remain. The reason for this behaviour is that the boundary condition for the numerical solution is not fulfilled by the analytical solution. Thus, the students learn that an error always can be expected when a front passes through an outflow boundary.

Sorption

Sorption denotes the interaction between the free pore space and the solid surfaces of the porous medium, on which a chemical component

can be attached due to various physical, chemical, biochemical or biological processes. Concerning the ‘speed’ of the interaction one distinguishes between fast and slow sorption. *Fast sorption* requires an extended form of equation (6), including the porous medium bulk density ρ_s , and the solid phase concentration c_s .

$$\frac{\partial}{\partial t}(\theta c + \rho_b c_s) + = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) \quad (9)$$

Differential equation (9) is not sufficient, because two unknown concentrations c and c_s appear. The formulation has to be completed by an equilibrium condition, which describes the relation between the two concentrations in case of equilibrium, the so-called isotherm $c_s(c)$. The name stems from the fact that it is measured for constant temperature. The three most important isotherms are:

- the linear isotherm $c_s = K_d c$
- the *Freundlich* isotherm $c_s = K_F c^N$
- the *Langmuir* isotherm $c_s = \frac{K_L \bar{c} c}{1 + K_L c}$

with parameters K_d , K_F , N , K_L and \bar{c} . COMSOL ESM allows all these options and parameters to be set easily with the relevant user interface for subdomain settings.

Using the equations for isotherms, the differential equation can be simplified to the following form:

$$\frac{\partial}{\partial t}(\theta R c) + = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) \quad (10)$$

with the so-called *retardation factor* $R > 1$ that, depending on the isotherm, is given by:

- $R = 1 + \frac{\rho_b}{\theta} K_d$ for the linear isotherm
- $R = 1 + \frac{\rho_b}{\theta} K_F N c^{N-1}$ for the Freundlich isotherm
- $R = 1 + \frac{\rho_b}{\theta} \frac{K_L \bar{c}}{(1 + K_L c)^2}$ for the Langmuir isotherm

The retarded transport with factor R delivers a simplified view of the influence of sorption, which is especially apparent in the case of the linear isotherm. For a homogeneous material and the linear isotherm there is a constant retardation factor R , whereas in the case of the other two isotherms R depends on the concentration c and thus varies in space and time even for a homogeneous porous medium.

As an exercise we chose a set-up that can be simulated in two ways: using the original sorption parameters to be entered in the ESM module (I) and by the retardation approach (II), based on equation . The model (II) is realised in COMSOL by selecting the time-scaling coefficient equal to R . To allow an easy comparison, we enter both set-ups as two different transport modes within one model. Fig. 4 depicts an exemplary student output.

By this exercise students realise that there is not only one possible model approach. Moreover, it becomes apparent that under certain conditions sorption processes lead to nothing else than retar-

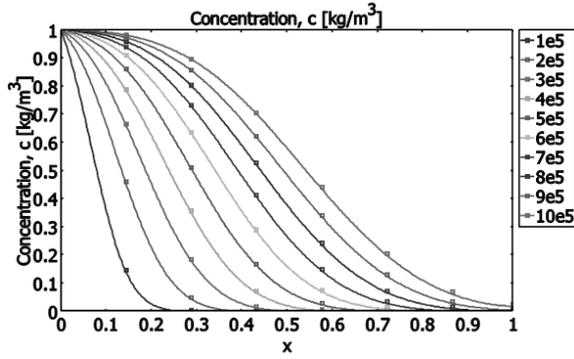


Fig. 4. Results for the sorption model, calculated by original ESM parameters ((I) in text, lines in the figure) and the retardation model ((II) in the text, markers in the figure); legend gives time instants in [s].

dation. Not to be underestimated is the sense of achievement for the participants, managing two different approaches, when the desired identical results appear on the display.

Degradation

If additionally degradation is taken into account, the differential equation (9) has to be extended to:

$$\frac{\partial}{\partial t}(\theta c + \rho_b c_s) = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) - \theta \lambda_f c - \rho_b \lambda_s c_s, \tag{11}$$

with decay constants λ_f for the fluid phase and λ_s for the solid phase. In case of linear sorption the differential equation can also be written as:

$$\frac{\partial}{\partial t} \theta \left(1 + \frac{\rho_b}{\theta} K_p \right) c = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) - \theta \lambda_f \left(1 + \frac{\rho_b \lambda_s}{\theta \lambda_f} K_p \right) c \tag{12}$$

The coefficient of c on the left side is the formerly introduced retardation factor R . The coefficient of c in the last term on the right side can be interpreted as another scaling factor σ , which is valid for decay only, whereas R is valid for storage.

$$\frac{\partial}{\partial t} \theta R c = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) - \theta \lambda_f \sigma c \tag{13}$$

If the decay constant is the same in both phases, the decay scaling factor is equal to R , which means that decay is not retarded:

$$\frac{\partial}{\partial t} \theta R c = \nabla \bullet (\mathbf{D} \nabla c - \mathbf{v} c) - \theta \lambda_f R c \tag{14}$$

For Langmuir and Freundlich isotherms similar considerations may apply. It has to be noted that coefficients R and σ both depend on c , i.e. they are spatially and temporally variable. Also for Langmuir and Freundlich isotherms it holds that R appears in both terms if the decay rates are the same in both phases.

The students compare breakthrough curves and profiles for different sorption and degradation settings. Most important are the post-processing COMSOL options for domain plot parameters and cross-section plot parameters. If these are used, even results from different model runs can be compared easily.

For the case of constant parameters the students also must compare with the analytical solution for retardation R and decay constant λ :

$$c(x, t) = \frac{c_{in}}{2} \left(\exp\left(\frac{v-u}{2D} x\right) \operatorname{erfc}\left(\frac{Rx-ut}{2\sqrt{DRt}}\right) + \exp\left(\frac{v+u}{2D} x\right) \operatorname{erfc}\left(\frac{Rx+ut}{2\sqrt{DRt}}\right) \right) \tag{15}$$

with $u = v + 4\lambda RD/v$ [5]. We demonstrate the student exercise for one example only. Parameters for the set-up are given in Table 1, all in a typical range for a column experiment. Almost all parameters can be entered directly. Only the decay term has to be specified indirectly: as liquid reaction term $-\theta \lambda_f c$ in ESM mode, or as reaction term $-\sigma \lambda_f c$ in the retardation approach according to equation (13). For the latter approach the retardation factor R is entered as time-scaling coefficient. From the parameters we obtain a retardation factor of 2. The time scaling factor σ introduced above is 1.

The results are shown in Fig. 5. Numerical parameters such as mesh spacing and accuracy are chosen in such a way that the output is mesh independent, i.e. there are no visible deviations between numerical and analytical results.

The comparison of numerical and analytical solutions fulfils several goals. First, it is similar to a test case for the software. It is checked whether the numerical and theoretical results agree. In case of disagreement all input parameters, physical and numerical, of the model have to be checked. If discrepancies still remain, one should examine, if conditions for both types of solutions are identical (see discussion of the

Table 1. Input parameters for the column experiment model

Parameter	Value [unit]	Parameter	Value [unit]
Porosity	0.25	Bulk density	1000 kg/m ³
Dispersivity	5 cm	Partition coefficient	0.25 10 ⁻³ m ³ /kg
Velocity	2.5 10 ⁻⁷ m/s	Decay rate in fluid	10 ⁻⁶ 1/s
Input concentration	1 g/l	Decay rate at solid	0
Initial concentration	0 g/l	Model length	1 m

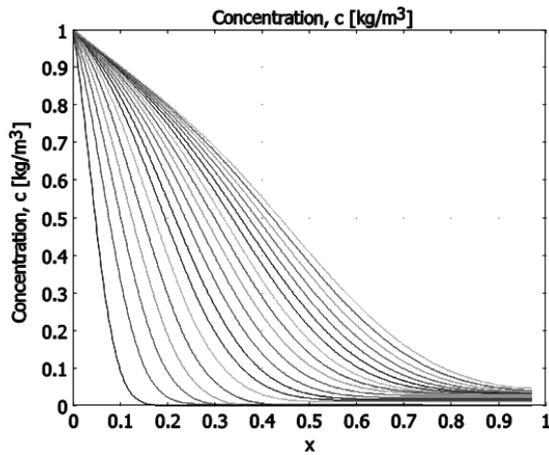


Fig. 5. Results for the numerical and analytical solutions for an advancing front of a degraded substance; there are no deviations visible, as parameters are chosen appropriately.

outflow boundary in the ‘Advection and dispersion’ section).

For the students, obtaining the aimed-for result confirms that they have understood how the software works. In addition it is instructive to see that there are several possibilities to work with the software and with differential equations. Such an understanding provides options for further work with more complex situations.

MULTIPHYSICS FLOW AND TRANSPORT

The students examine one 2D example in which flow and transport are linked. It is their first real multiphysics model. Point of origin is a situation, in which there is a local contamination within an aquifer. The students are asked to set up a model to answer the question, if the concentration at the outflow boundary remains below a limit concentration within one year after a hypothetical accident that caused the contamination.

The steady-state flow field has to be modelled using Darcy’s Law. There are no-flow (Neumann) conditions and given head (Dirichlet) conditions at different parts of the boundary. After the flow model has been set up, the transport model is added, using the COMSOL ‘esst’ mode from ESM. The exact location and extension of the contamination are given, and there are the following input parameters: initial concentration, longitudinal and transversal dispersivities, molecular diffusivity, tortuosity and porosity. In this case all boundary conditions for the concentration are of no-flow type, which can be entered most easily by COMSOL as ‘advective flux’. The major step for understanding the multiphysics concept is the connection between both modes, which is performed by entering the velocities from the ‘esdl’ mode in the appropriate input box of the ‘esst’ mode. The problem is treated in two steps. It is first solved for flow, in the steady state mode, as

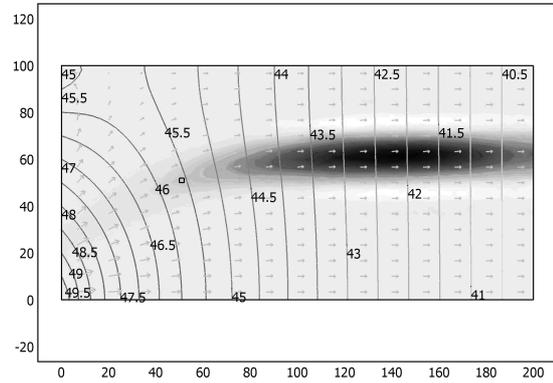


Fig. 6. Contamination plume example for flow and transport modelling.

the flow is assumed to be constant. In the second step students switch to the transient solver mode to solve for transport only. To perform these two steps correctly, the ‘Solver Parameters’ have to be set and the ‘Solver Manager’ has to be handled appropriately.

The graphical output of the example is given in Fig. 6, which depicts the concentration as surface plot, the velocity field as arrows, and the isobars as contour lines. A black rectangle indicates the location of the original contamination. In the figure various features of the plume behaviour are nicely visible: the plume moves with the advection field and spreads mostly in the direction of flow, and less pronounced transverse to it.

COUPLED FLOW AND TRANSPORT

In the first multiphysics exercise, described in the previous section, the two COMSOL modes for flow and transport could be solved separately. The steady state flow field was determined in a first step, and the contaminant transport could be simulated in a second step. That solution procedure was possible because the connection between the modes is one-way only, from flow to transport. In the exercise the two modes can be solved in a single COMSOL run, but this was not necessary. In this section we present a more complex situation in which the simultaneous solution of the two modes is required, and the solution cannot be solved in two separate steps, because the modes are coupled.

In the literature the term coupling refers to the situation in which flow and transport are mutually connected. While there is always a link from flow to transport, the link from transport to flow is given if fluid properties, density and viscosity, are affected by the transport variable. In practice salinity or temperature are such variables that affect fluid properties. If there is an influence on density only, we speak of density-driven flow [2, 6].

The Henry example is a classical test case for codes to model density-driven porous media flow [2, 7, 8, 9, 10, 11, 12]. It is a simplified model for the description of seawater intrusion into a fresh-

Table 2. Input parameters for the Henry saltwater intrusion problem

Parameter	Value [unit]	Parameter	Value [unit]
Length	200 m	Inflow velocity	$6.6 \cdot 10^{-3}$ m/d
Height	100 m	Porosity	0.35
Freshwater density	1000 kg/m ³	Dispersivities	0 m
Seawater density	1025 kg/m ³	Diffusivity	0.1886 m ² /d
Hydraulic conductivity	1 m/d	Tortuosity	1

water coastal aquifer, a very relevant problem in practical hydrogeology. The model region represents a vertical cross-section through a coastal aquifer, with fixed freshwater inflow at one side and seawater concentration at the other side. For the model we do not use the original dimensionless variables but a modified dataset, which is equivalent to the original data. The input values are given in Table 2 and are identical to those given by Ségol [13]. There is a linear change of density with salinity in the relevant range for seawater intrusion. Temperature effects on density are neglected. For the COMSOL model we again use the 'esdl' and 'esst' modes of the ESM. Coupling variables are the velocities (from 'esdl' to 'esst') and density (from 'esst' to 'esdl').

Fig. 7 depicts results for the Henry test case. The seawater side is shown on the right side of the plot. The figure shows the density distribution, dependent on the salinity distribution, within the cross-section. Saline, high-density fluid is depicted in dark, freshwater in light colour. The flow field is represented by an arrow field. Contour lines are used to visualise isobars. There are also streamlines created by specification of start positions at the seawater side boundary.

Streamlines show that the saline water, entering the aquifer from the seawater side in the lower part of the aquifer, mixes with the freshwater from the opposite side. With salinity decreasing, the density is also reduced causing the water to rise gradually due to buoyancy. Along the streamlines, which originate at the seawater side, at a certain position the horizontal velocity becomes zero and changes the sign, i.e. the streamline turns back towards the sea. The behaviour described by a numerical model, is observed in real systems, not only in aquifers but also within coastal waters.

CONCLUSIONS

COMSOL Multiphysics is used in a course on groundwater modelling, in order to enhance students' understanding of the relevant flow and transport processes and to the use experience of a user-friendly software tool for numerical modeling. The students benefit from the easy handling of model input, which is performed completely within the graphical user interface. There is no need to use a programming language. Most striking are the post-processing options, which allow visualisation

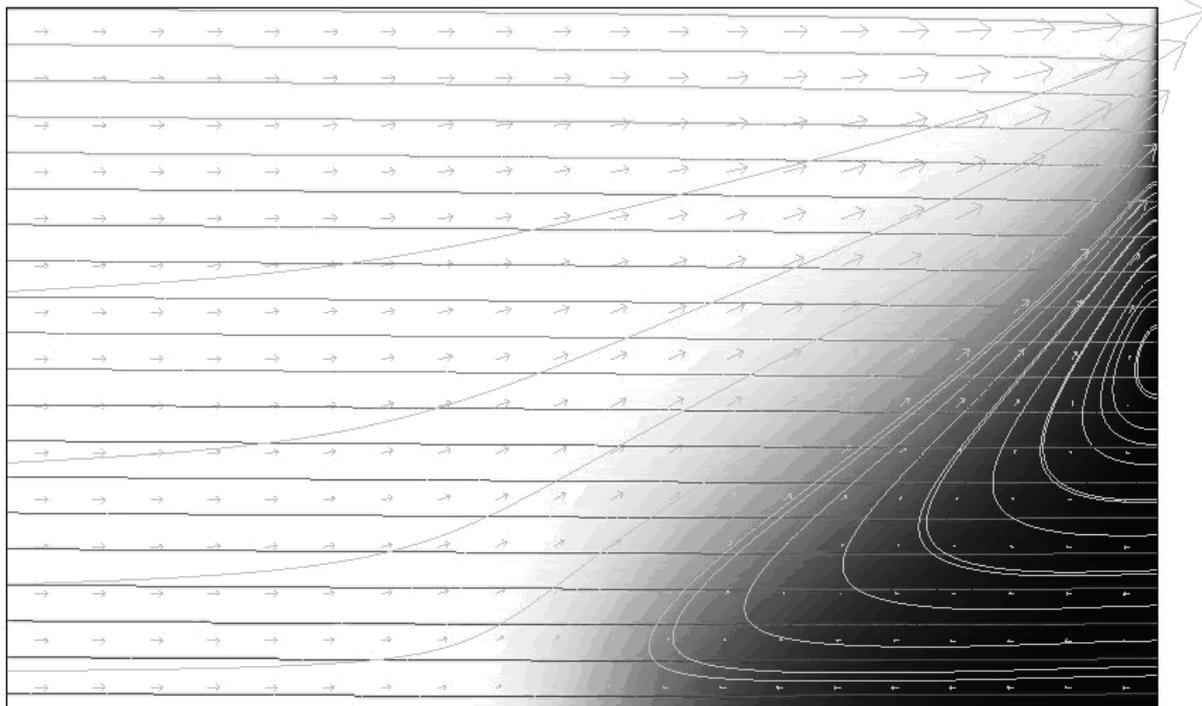


Fig. 7. The Henry test case for saltwater intrusion, a coupled flow and transport problem.

of the temporal development (breakthrough curves) and the spatial distribution (profiles), not only from a single model run but from several runs. In addition an impression of both the temporal and spatial development of a variable can be gained by using the COMSOL animation option.

Students learn:

- how to use a user-friendly graphical user interface of a complex simulation tool;
- what is a model region and what are boundary conditions;
- which types of boundary conditions can be selected;
- what are appropriate formulations for different aquifer settings;
- what are basic features of transport, degradation and sorption;
- that sorption is equivalent to retardation under certain conditions (which are fulfilled in simple cases);
- that there are various options to reduce errors from the numerical method;
- that some deviations between analytical and numerical solutions remain, as they stem from different assumptions concerning the physics of the situation;
- that there is a link from flow to transport;
- that flow and transport are coupled if the transport variable has an influence on the fluid properties;

- that solutions can be improved by reducing required solver accuracy, and by refining the mesh;
- that transport solutions may have to be improved by options concerning artificial diffusion;
- how to compare results from different model runs.

The basic features of the transport-sorption-degradation system can be examined best for the simple 1D set, representing a column experiment.

A stepwise introduction of flow modelling, transport simulation, one-way linked flow and transport, and two-way coupled flow and transport illustrates the basic features of the multi-physics approach. For such an aim COMSOL is the perfect software, as all types of connections between the physical modes can be accessed and manipulated by the user. Here, due to its multi-physics concept, the program is superior to other software.

The Earth Science module (ESM) for COMSOL Multiphysics is an efficient tool that enables earth science students to transfer real world hydrogeological systems into numerical models. However, some features need improvement to make ESM competitive with professional software that is especially designed for groundwater flow and transport modelling.

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