A FEM - based Approach to ARGESIM Benchmark C19R 'Pollution in Groundwater Flow' using COMSOL Multiphysics

Harald Teufelsbauer, University of Natural Resources and Applied Life Sciences, Vienna

harald.teufelsbauer@boku.ac.at

Simulator: *COMSOL Multiphysics* is a modelling package for the simulation of a wide range of physical processes one can describe with partial differential equations (PDEs). COMSOL offers the opportunity to interact with *MATLAB*. Functions which are defined in MATLAB can directly be called in COMSOL if MATLAB is working in the background. The modelling of most phenomena can be done easily through predefined templates. Modifying these to specific applications is possible through equation-based modelling capabilities.

Modelling. The groundwater flow can be modelled with a transport equation, describing convection and diffusion processes. COMSOL Multiphysics offers a predefined template which is suitable for modelling this task. The equation offered is

$$\delta_{ts}\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - u \cdot \nabla c$$

COMSOL allows solving the transport equation for one- up to three-dimensional geometries. To solve the task of groundwater flow rectangle geometry is used. COMSOL offers a very user-friendly GUI, where also more complex two-dimensional geometries can be drawn by combination of circles, ellipses, rectangles, lines and 2nd and 3rd degree Bezier curves.

Figure 1 shows the meshed rectangle geometry used for the simulations. The steady source of pollutant *M* is placed at the point (0, 0). As COMSOL does not support the definition of concentrations or fluxes on singular points, the pollution source is realised by a little hole with an arbitrary chosen radius, e.g. $r_M = 0.2$ m. A triangular mesh can be generated by one simple mouse click. If necessary, a user controlled mesh generation can be defined in a mesh setting menu. Local mesh refinements can be done very simple, by marking the desired area with the mouse and clicking a refinement button. The domain consists of one big rectangle rigged by the pollution source (subdomain). Two cycles define two further subdomains, describing the facilities used for task B and task C. The properties of these subdomains can be treated separately. The subdomain setting mask (Figure 5) allows defining the PDE's coefficients and the initial values of each subdomain.

The boundaries can be treated by dint of the boundary settings mask, where different kinds of boundary conditions can be selected.
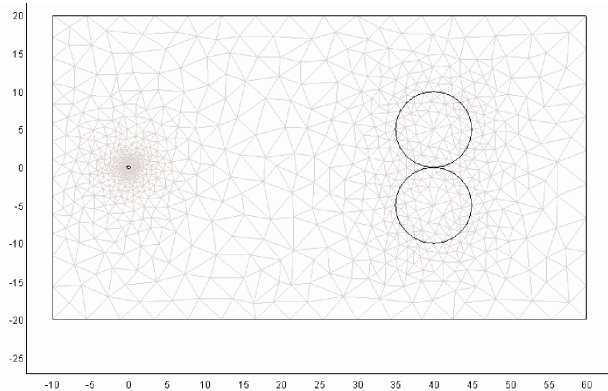

Figure 1: Model geometry and finite element mesh with refinements at pollutant source *M* an around facilities for pollution depletion.

On each selected margin the boundary conditions fulfiling the transport equation can define a forced concentration or a flux through the boundary. The right boundary of the rectangle is allocated to a flux condition, whereas the inward flux is zero.

The other boundaries of the rectangle use convective flux conditions, which assume that all mass passing through these boundaries is convection – dominated. This is useful in convection-dominated mass balances where the outlet concentration is unknown. The source of pollutant M is defined by dint of a flux boundary condition, provided by COMSOL where the right hand side describes the user defined incoming flux, respectively the pollution:

$$-\vec{n} \cdot (-D\nabla c + c\vec{u}) = \frac{M}{h \cdot n_e \cdot 2r_M\pi}$$

A - **Task: Simulation of Unaffected Pollution Spread. C**OMSOL provides a number of different solvers and solver settings. All tasks of this comparison are solved using an UMFPACK solver with a relative tolerance of 10^{-5}.

Figure 2 and Figure 3 show results for time steps $t = 50$ and $t = 100$. The solution of time step $t = 150$ fits exactly to the solution at $t = 100$. The accuracy of the FEM solution can be increased especially by the mesh fineness and its quality. The analytical approximation is calculated in MATLAB, called directly from COMSOL Multiphysics in a subdomain definition window.
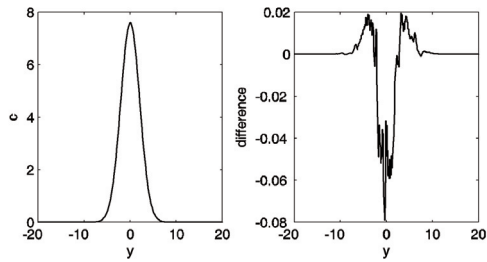
Figure 2: FEM solution at $(50, y)$, $t = 50$ (plot at left) and difference analytical / FEM solution (plot at right).
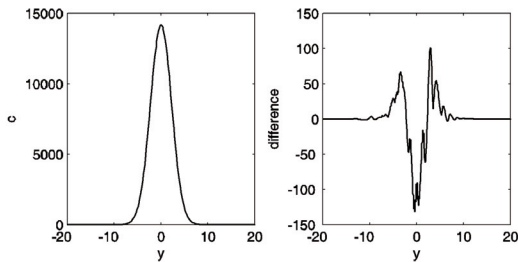

Figure 2: FEM solution at $(50, y)$, $t = 100$ (plot at left) and difference analytical / FEM solution (plot at right).

B - **Task: Pollution Reduction by Facilities.** COMSOL is able to derive the steady state solution of the transport equation numerically. This solution can be used as initial value of the following time dependent solving process, by using the restart-button instead of the solve-button. Before the time dependent solution can be started with switched-on plants, the reaction rate R in the subdomain settings of the two circles have to be changed from zero to $-\lambda \cdot c$ (Figure 5; numerical solutions given in Figure 4).

C - **Task: Controlled Pollution Reduction.** If the facilities are periodically active, Monday to Friday from 20.00 - 08.00, and at weekends around the clock, the reaction rate can be controlled by a MATLAB script function. COMSOL is able to handle this function by calling it in the subdomain settings. The MATLAB function `reaction.m` is called in the reaction rate input line of the subdomain setting mask (Figure 5). Numerical results are given in Figure 6.
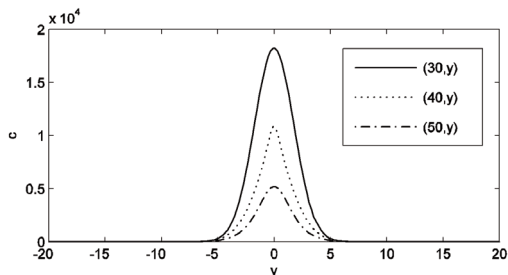

Figure 4: Concentration at the lines $(30, y)$, $(40, y)$, $(50, y)$ at $t = 100$ days, with continously working pollution reduction facilities
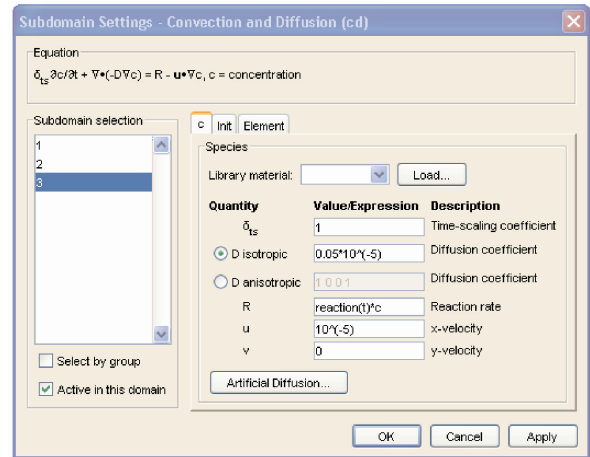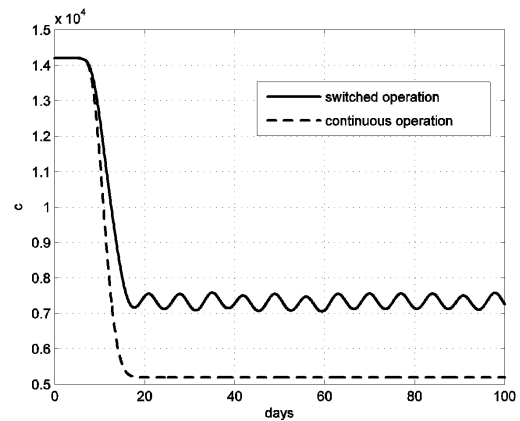

Figure 5: Definition mask for subdomain dynamics.

Figure 6: Concentration at $(50, 0)$ for $0 \le t \le 100$ days with pollution reduction facilities, continuous and switched operation.

Résumé: This solution with COMSOL Multiphysics is based on the Finite-Element - Method (FEM). The groundwater stream is modelled as (finite) rectangle, with subdomains for the source and for the two facilities. On each subdomain, refined grids and suitable boundary conditions are used, in order to calculate a solution with a suitable solver (UMFPACK). The approximation for the solution, the continuous degradation for the plant activities, and time control for the plant operation are modelled by MATLAB functions, to be called directly from COMSOL Multiphysics. For this solution, COMSOL Multiphysics 3.1 has been used.

Corresponding Author:
Harald Teufelsbauer, *harald.teufelsbauer@boku.ac.at*
Department of Structural Engineering & Natural Hazard,
Institute of Mountain Risk Engineering,
University of Natural Resources and Applied Life Sciences
Peter Jordan - Strasse 82, 1190, Vienna, Austria