Variable dependant boundary condition benchmark

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1 Analytical Solution

The component transport process is used for the benchmark setup. Here, a analytical solution of a simple setup is derived and compared to the numerical results. Please see the process documentation for detailed derivation of the underlying equations.

1.1 Reduction of Problem Complexity

The component transport process is based on a system of PDEs, which can be categorized in equations describing the groundwater flow, and equations for the component transport. The groundwater flow is described by

$$\phi \frac{\partial \rho_R}{\partial p}\frac{\partial p}{\partial t} + \phi \frac{\partial \rho_R}{\partial \omega_C}\frac{\partial \omega_C}{\partial t} - \operatorname{div}\left(\frac{\boldsymbol{\kappa}}{\mu}\rho_R\left(\nabla p - \rho_R g\right)\right) + Q_p = 0.$$

The component transport is described by

$$\omega_C R\phi \frac{\partial \rho_R}{\partial p}\frac{\partial p}{\partial t} + \omega_C R\phi\left(\frac{\rho_R}{\omega_C} + \frac{\partial \rho_R}{\partial \omega_C}\right)\frac{\partial \omega_C}{\partial t} - \operatorname{div}\left(\frac{\boldsymbol{\kappa}}{\mu}\rho_R\omega_C\left(\nabla p - \rho_R g\right) + \rho_R \mathbf{D}_h \nabla \omega_C\right) + Q_{\omega_C} + R\theta\phi\rho_R\omega_C = 0.$$

If the density ρ_R is assumed to be constant and in the absence of sources the equations simplify to

$$-\operatorname{div}\left(\frac{\boldsymbol{\kappa}}{\mu}\left(\nabla p - \rho_R g\right)\right) = 0,$$

and

$$R\phi\frac{\partial \omega_C}{\partial t} - \operatorname{div}\left(\frac{\boldsymbol{\kappa}}{\mu}\omega_C\left(\nabla p - \rho_R g\right) + \mathbf{D}_h\nabla\omega_C\right) = 0.$$

in the case of absence of gravity ($g = 0$), vanishing diffusion and dispersion ($\mathbf{D}_h = 0$) and a constant ratio of permeability and viscosity $\left(\frac{\kappa}{\mu} = A = \mathit{const.}\right)$ the system further simplifies to

$$-\operatorname{div} A\left(\nabla p\right) = 0, \tag{1.1}$$

and

$$R\phi\frac{\partial \omega_C}{\partial t} - A\operatorname{div}\left(\omega_C\nabla p\right) = 0. \tag{1.2}$$

Using (1.1) in (1.2), Equation (1.2) further simplifies to

$$R\phi\frac{\partial \omega_C}{\partial t} - A\nabla p\operatorname{div}\left(\omega_C\right) = 0. \tag{1.3}$$

1.2 Analytical Solution for Benchmark Scenario

In one dimension, we apply on as boundary conditions for a system of size 1

$$\omega_C(0,t) = 2 \tag{1.4}$$

$$p(0,t) = 1 \tag{1.5}$$

$$\langle A\rho_R \nabla p(1,t)|n\rangle = A(\omega_C(1,t) - 1) \tag{1.6}$$

$$\langle A\rho_R \omega_C(1,t)\nabla p(1,t)|n\rangle = \langle A\omega_C(1,t)\nabla p(1,t)|n\rangle, \tag{1.7}$$

and the initial conditions

$$p(x,0) = 1 - x \tag{1.8}$$

$$\omega_C(x,0) = \lambda(x-1). \tag{1.9}$$

From (1.6), (1.8) and (1.9) we see immediately, that $\nabla\omega_C(1,t) = \lambda$ at the right boundary for all times t.
For this system, the analytical solution for the concentration at the right boundary reads

$$\omega_C(1,t) = \exp\left(-\frac{A\lambda}{\phi R\rho_R}t\right) - 1 \tag{1.10}$$

1.3 Comparison of Analytical and Simulation Results

For the setup, the parameters are choosen as

$$A = 10^{-3} \tag{1.11}$$

$$\lambda = -2 \tag{1.12}$$

$$\phi = 10^{-1} \tag{1.13}$$

$$R = 1 \tag{1.14}$$

$$\rho_R = 10^3 \tag{1.15}$$

The comparison of analytical and numerical results for widest time stepping of 10 and grid spacing of 0.1 is shown in Figure 1.3.
According to the results of table 1.3 which shows the maximal relative error of simulation results for different time and space spacings, for the benchmark project file time stepping is choosen as 10 and grid spacing as 0.1. This leads to a good tradeoff for accuracy and computation cost.

$\bullet$	$\Delta t \approx 1$		$\Delta t \approx 10$		$\Delta t \approx 50$	
$\Delta x = 0.01$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-5}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-4}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 5\times 10^{-4}$
$\Delta x = 0.1$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 5\times 10^{-5}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-4}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 5\times 10^{-4}$
$\Delta x = 0.5$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-1}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-1}$	$\frac{\omega_C^n(t)-\omega_C^a(t)}{\omega_C^a(t)}$	$< 1\times 10^{-1}$

Table 1.1: Relative error for different grid and time spacings.

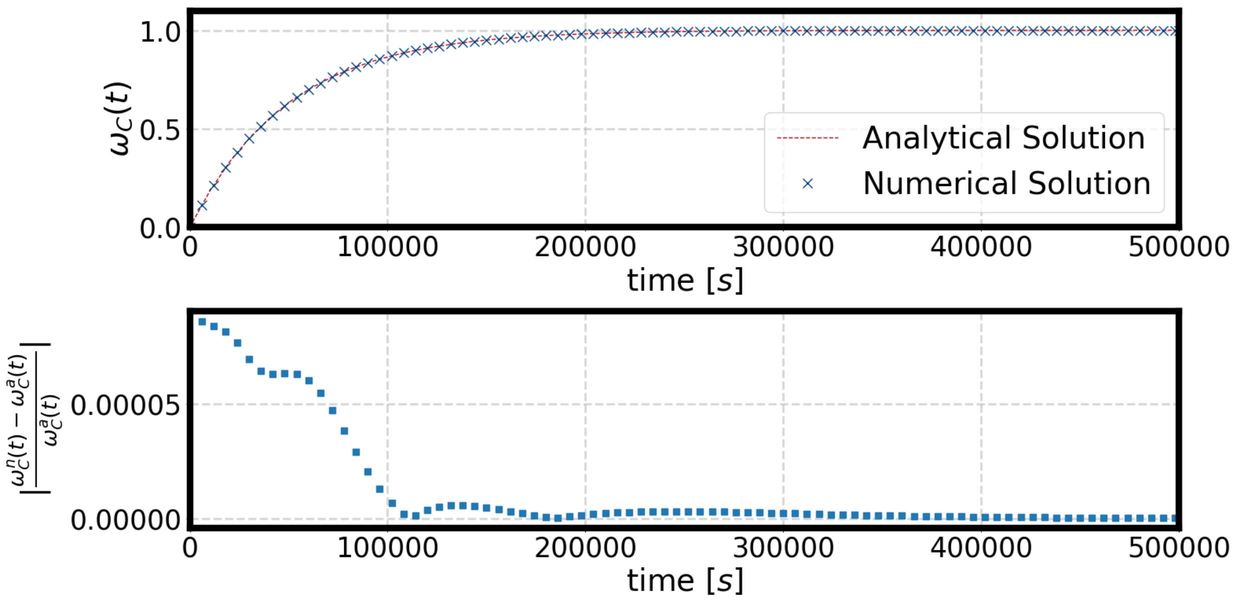

Figure 1.1: *upper part:* Analytical solution on the right boundary in dependance of time t of the problem indicated with red dashed line in comparison to numerical solution indicated by blue crosses, *lower part:* development of relative error in dependance of time t. Grid spacing for simulations: 0.1; widest timestep 10. The relative error is below 5×10^{-5} for all simulation times.