Numerical modelling of solute flow dispersion in porous media using simulator MUFITS

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Abstract. An extension of the MUFITS reservoir simulator for modelling solute transport in a porous medium is presented. The new option concerns modelling of the longitudinal and transverse mechanical dispersion of the solute flow. The numerical dispersion coefficients for the solute transport are derived. The sufficient condition for the time step and the grid resolution that ensure accurate modelling of mixing in porous media is presented. Two benchmark problems which allow exact analytical solution are described and are used for validation of the developed simulation option. The solute distributions calculated with MUFITS are in a good agreement with the exact solutions.

1. Introduction
Flows in porous media occur in many practical applications related to the Earth’s subsurface exploration and utilization. In particular, such flows in geological permeable reservoirs develop in the processes of oil and gas recovery [1,2], subsurface sequestration of greenhouse gases [3,4], underground gas storage [3,5], recovery of geothermal energy [6], and many others. These applications include complicated flows which are often multiphase, multicomponent and non-isothermal, and are under the influence of variety of physical phenomena. All the phenomena can be taken into account only in numerical simulations which on its own require development of complicated computer programs that are called the reservoir simulators. The validation of the simulators accuracy is done by means of benchmarking against test problems which, for example, allow exact analytical solutions.

This work concerns ongoing development of the MUFITS reservoir simulator [7]. It includes different models for transport in porous media, in particular the Black-oil model [2,8], the model for binary mixture flows in a wide range of pressures and temperatures with account for liquid-liquid-gas phase equilibria [4,9], and other models [10]. The functionality of MUFITS allows engineering 3D simulations with detailed data for geological structure of subsurface reservoirs, fluid and rock properties, well operational controls, initial hydrostatic equilibria of multiphase fluids, and others.

Here we present a new simulation option of the simulator for modelling the mechanical dispersion of solute transport in porous media [11,12]. The dispersion results in mixing of solute transported through the media which occurs on the pore scale due to chaotically changing velocities and flow paths of fluid particles (figure 1) even if porous media are homogeneous on the macroscale. As a result of the velocity field perturbations some particles travel faster than the others and choose different paths when flowing around the skeleton grains. As a consequence, two particles located close to each other at an initial time are dispersed both along and across the mean flow direction.
Figure 1. A schematic microscale view of mechanical dispersion in a porous medium which skeleton is shown in grey color. Instantaneous stream lines are shown (a–d). The mean flow direction is from left to right.

Farther we describe the equations utilized in the code for the mechanical dispersion in single-phase two-component flows and discuss its order of approximation with the finite-difference scheme used in MUFITS. We also present two benchmark problems which allow exact solutions and we validate the simulator against these problems.

2. Governing equations
Let us consider isothermal single-phase flow of a two-component fluid in a homogeneous isotropic porous medium. The flow is governed by the equations [9,11,12]

\[ \frac{\partial}{\partial t}(\phi \rho) + \text{div}(\rho \mathbf{u}) = 0 \]  
\[ \frac{\partial}{\partial t}(\phi c) + \text{div}(\rho c \mathbf{u}) = \text{div}(\phi \rho \mathbf{D} \text{grad} c) \]  
\[ \mathbf{u} = -\frac{K}{\mu} \text{grad} P \]

where \( \phi \) is the porosity, \( \rho \) is the fluid density, \( \mathbf{u} \) is the Darcy’s velocity, \( c \) is the mass concentration of the solute component which is assumed small (\( c \rightarrow 0 \)), \( \mathbf{D} \) is the tensor of mechanical dispersion, \( K \) is the permeability, \( \mu \) is the fluid viscosity, and \( P \) is the pressure. The equations (1) and (2) are the mass balance equations for the bulk fluid and the solute component, respectively, and (3) is the Darcy’s law.

The dispersion tensor is given by the following matrix

\[ \mathbf{D} = \frac{1}{\phi} \begin{pmatrix} \lambda_L u_x + \lambda_T (u_y + u_z) & 0 & 0 \\ 0 & \lambda_L u_y + \lambda_T (u_z + u_x) & 0 \\ 0 & 0 & \lambda_L u_z + \lambda_T (u_x + u_y) \end{pmatrix} \]

where \( \lambda_L \) and \( \lambda_T \) are the longitudinal and transverse mean free path of a small volume of fluid caused by mixing in porous medium [11]. The length \( \lambda_L \) (or \( \lambda_T \)) is the mean distance at which two initially close particles scatter along (or across) the mean direction of flow.

Assuming that the fluid is incompressible (\( \rho = \text{const} \)) the equations (1) and (2) reduce to

\[ \text{div}(\mathbf{u}) = 0 \]
Substituting the relations (3) and (4) in the equations (5) and (6) we get a closed system on $P$ and the solute concentration $c$.

3. About numerical dispersion

Numerical solution of the system (5) and (6) results in solute dilution due to numerical dispersion. Thus, the simulator calculates the transport in accordance with the equation (7) rather than (6).

$$ \frac{\partial c}{\partial t} + \frac{u}{\phi} \text{grad} c = \text{div} \left( D \text{grad} c \right) $$

Here $D_{num}$ is the tensor of the numerical dispersion. If the transport is simulated with the fully implicit upwind scheme [13] of the first order of approximation, which is the standard method for reservoir simulations and is utilized in MUFITS, then $D_{num}$ is given by

$$ D_{num} = \frac{1}{\phi} \begin{pmatrix} h_{i}u_{x} + \tau_{i}u_{x}^{2} & \tau_{i}u_{y} & \tau_{i}u_{z} \\ \tau_{i}u_{x} & h_{i}u_{y} + \tau_{i}u_{y}^{2} & \tau_{i}u_{z} \\ \tau_{i}u_{x} & \tau_{i}u_{y} & h_{i}u_{z} + \tau_{i}u_{z}^{2} \end{pmatrix} $$

where $h_{i}$ is the grid block length along axis $i = x, y, z$ and $\tau$ is the time step.

For accurate numerical modelling the absolute values of the elements of the matrix $D_{num}$ should be much less than the absolute values of the elements $D$. The sufficient condition for this can be written as

$$ h_{i} \ll \lambda_{L}, \quad |u_{i}| \ll \lambda_{L}, \quad \tau u_{j} \rightarrow 0 $$

4. Benchmark problem

Let us consider a 1D problem of the two-component fluid flow along axis $x$ ($x \in (-\infty, +\infty)$), i.e., $u_{y} = 0$, $u_{z} = 0$. Then, from the equation (5) we obtain $u_{x} = \text{const}$, whereas (6) reduces to

$$ \frac{\partial c}{\partial t} + \frac{u}{\phi} \frac{\partial c}{\partial x} = D_{L} \frac{\partial^{2} c}{\partial x^{2}}, \quad D_{L} = \lambda_{L}u_{x} = \text{const} $$

At the initial moment of time the concentration distribution along $x$ is a stepwise function $c(x)$ with a discontinuity at $x = 0$:

$$ t = 0: \quad c = \begin{cases} c_{0}, & x \leq 0 \\ 0, & x > 0 \end{cases} $$

where $c_{0}$ is a constant.

The problem (10) and (11) allows exact solution in the form

$$ c(x,t) = \frac{c_{0}}{2} \left[ 1 - \text{erf} \left( \frac{x - u_{x}/\phi t}{2\sqrt{D_{L}t}} \right) \right], \quad \text{erf}(\xi) = \frac{2}{\sqrt{\pi}} \int_{0}^{\xi} \exp(-a^{2}) \, da $$

where $\text{erf}(\xi)$ is the error function.
For numerical solution of this problem with MUFITS, we simulate, using the GASSTORE module [5], the isothermal flow of brine (NaCl–H₂O mixture) in the domain \( x \in [x_{\min}, x_{\max}] \), where \( x_{\min} = -20 \) m and \( x_{\max} = 100 \) m. The water salinity is small, \( c_0 = 10^{-4} \), thus its variations do not significantly change the brine density \( \rho \). The rock properties are \( \phi = 0.1 \), \( K = 100 \) mD, \( \lambda_L = 1 \) m, and \( \lambda_F = 0 \) m. The initial pressure is 50 bar. The density and viscosity of water for a given \( P \) and constant reservoir temperature of 50°C are calculated using accurate correlations from the paper [13]. The brine of salinity \( c_0 \) is injected into the domain through the boundary \( x = x_{\min} \) with the relative injection rate of \( 10^{-4} \) ton/day·m², and the initial pressure is maintained at the boundary \( x = x_{\max} \). The flow is simulated over the time \( t \in [0, t_*] \), where \( t_* = 5 \cdot 10^4 \) days. Since the injection rate is small, the pressure in the whole domain does not significantly deviate from its initial value. Particularly, the pressure at the boundary \( x = x_{\min} \) rises due to brine inflow through that boundary but it does not exceed \( P = 50.01 \) bar. Thus, taking into account that salinity variation is also small, the assumption of incompressible flow is hold in the numerical modelling of the benchmark problem. The boundaries of the domain \( x_{\min} \) and \( x_{\max} \) are placed far enough from the central region where \( c \) changes significantly in order not to influence \( c \) distribution. The flow is simulated with a uniform grid of 12000 elements and the maximum timestep is constrained by 7.5 days.

The simulation results are shown in figure 2 for successive times \( t = 0, 0.25t_*, 0.5t_*, 0.75t_*, \) and \( t_* \). The solid lines show the exact solution (12), where \( u_* = 10^{-4} \) m/day. The symbols correspond to the numerical solution calculated with MUFITS. The numerical solution matches the exact solution what validates correctness of implemented in the simulator numerical algorithms for modelling longitudinal dispersion.

![Figure 2. Comparison between exact and numerical solution of the benchmark problem 1.](image)

5. Benchmark problem 2
Now, we consider a 2D problem of steady flow along axis \( x \) \( (u_y = 0, u_z = 0) \) in the region \( x \geq 0, y \in (-\infty, +\infty) \). Then, from the equation (5) we obtain that \( u_x = \text{const} \), whereas assuming that \( \lambda_L = 0 \) the equation (6) reduces to
The fluid with constant $c = 0$ (or $c = c_0$) and $u_x = \text{const}$ is injected into the domain through the boundary $x = 0$:

$$x = 0: \quad c = \begin{cases} c_0, & y > 0 \\ 0, & y \leq 0 \end{cases}$$

(14)

According to (10) brines of different salinities are injected into the layers $y > 0$ and $y \leq 0$.

The problem (13) and (14) allows exact solution

$$c(x, y) = \frac{c_0}{2} \left( 1 - \text{erf} \left( \frac{y}{2\sqrt{\lambda_T x}} \right) \right)$$

(15)

which describes solute mixing due to transverse dispersion in porous medium. According to (11), the sharp at $x = 0$ boundary between fluids of different concentrations $c$ becomes increasingly blurry with rising $x$.

For numerical solution of this problem with MUFITS, we simulate the isothermal (at $T = 50^\circ C$) flow of brine (NaCl–H$_2$O) in the domain $x \in [x_{\min}, x_{\max}]$, $y \in [y_{\min}, y_{\max}]$, where $x_{\min} = 0$ m, $x_{\max} = 100$ m, $y_{\min} = -15$ m, and $y_{\max} = 15$ m. The water salinity is small, $c_0 = 10^{-4}$, thus its variation due to dispersion does not significantly change the density $\rho$. The porous skeleton properties are $\phi = 0.2$, $K = 100$ mD, $\lambda_L = 0$ m, and $\lambda_T = 0.1$ m. The pressure at the boundaries $x = x_{\min}$ and $x = x_{\max}$ is maintained at $P = 55$ bar and $P = 54.96$ bar respectively. Therefore, pressure does not significantly change and, taking into account that salinity variations are small, the assumption of incompressible flow is hold in numerical modelling. The impermeable boundaries $y = y_{\min}$ and $y = y_{\max}$ are set far enough from the region of $c$ variations due to transverse dispersion in order not to influence the $c$ distribution. The problem is simulated with a uniform rectilinear grid of 200 by 120 elements along axes $x$ and $y$, respectively, until $t = 10^5$ days when the steady flow is reached.

![Contour lines of solute concentration](image)

Figure 3. Contour lines of solute concentration $c$ in the numerical solution of the test problem 2. Eleven contours with uniform step are shown in the range $c \in [10^{-6}, 9.9 \cdot 10^{-5}]$

The simulation results are shown in figure 3. The contour lines of the concentration $c$ given by (15) are shown. At $x = x_{\min}$ the boundary between the fresh water injected at $y > 0$ and the brine injected at $y \leq 0$ is sharp. This boundary becomes increasingly blurred downstream due to mixing in the transverse direction to the flow. The numerical and exact solutions at $x = x_{\max}$ are compared in figure 4. There is a good match between the solutions what validate correctness of the numerical algorithms for modelling transverse dispersion implemented in the simulator.
6. Conclusions

A new simulation option of the MUFITS reservoir simulator for modelling mechanical dispersion in porous media has been developed. The sufficient conditions for the time step and grid resolution that ensure an accurate modelling of the solute transport with MUFITS has been derived. The option validation against two benchmark problems concerning solute dispersion in a porous medium demonstrates correctness of the option implementation in the simulator program code.

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