

Numerical modelling of convectio-diffusion-adsorption problems in 1D using dynamical discretization

J. Kačur, B. Malengier, E. Trojaková

Extended abstract

We consider a convection-diffusion-adsorption-reaction system in 1D, which models contaminant transport in groundwater. Mathematical model is numerically solved by the method of line (MOL) using the space discretization with the moving grid points. The method is suitable to capture the sharp fronts of the solution which can arise by a strong adsorption. The large scale of isotherms are included in the adsorption model for both equilibrium and nonequilibrium modes. Also the numerical approximation by operator splitting method is applied when adsorption process is splitted with the convection-diffusion along the short time intervals and the fixed space grid points. The numerical efficiency of all methods is discussed and obtained numerical results are compared. The presented methods are suitable for the solution of inverse problems in scaling of the mathematical model for its practical implementations.

The contaminant transport in porous media is modelled (see [5, 2], etc.) by system of PDE's in the following form:

$$\begin{aligned} \theta \partial_t C + \rho \partial_t \psi_e(C) + \theta \mathbf{v} \nabla C - \nabla(\theta \mathbf{D} \nabla C) + \rho \partial_t S &= 0 \\ \partial_t S &= \kappa(\psi_n(C) - S) \end{aligned} \quad (1)$$

eq1.1

where C is the contaminant concentration, θ, ρ are porosity and specific density of the porous media, \mathbf{v} is the water flow in which contaminant is soluted, and ψ_e, ψ_n are adsorption isotherms in the equilibrium and nonequilibrium mode, respectively. The matrix \mathbf{D} represents the dispersion. System (1) can be completed by an initial and boundary conditions which will be specified below. The adsorption phenomenon is characterized by adsorption isotherm - a function that relates the amount of adsorbed material to its amount in the water when the equilibrium state is reached. Different adsorbate-adsorbent pairs can have different isotherms. The most common isotherms (ψ_e, ψ_n) used in practice are:

Linear isotherm - $\psi(C) = aC$

Freundlich isotherm - $\psi(C) = aC^p$

Langmuir isotherm - $\psi(C) = \frac{aC}{1+bC}$

Mixed F-L isotherm - $\psi(C) = \frac{aC^p}{1+bC^p}$

Lindstrom-Van Genuchten isotherm $\psi(C) = aCe^{-2b\psi(C)}$.

If $\kappa \rightarrow \infty$ (case of equilibrium adsorption mode) then $S = \Psi_n(C)$ and then we can add $\partial_t \Psi_n(C)$ to the parabolic term. Thus, $\partial_t \Psi_e(C)$ in (1) represents the adsorption part in equilibrium mode. The porous medium can be a composition of various materials. That means that while some compounds adsorb the contaminant in equilibrium mode, the other ones may adsorb in nonequilibrium mode or need not adsorb at all. Thus, (1) represents the transport of contaminant in porous media with (reversible) adsorption in equilibrium and nonequilibrium mode. If in (1) the term $\partial_t S$ is of the form

$$\partial_t S = \kappa \max(0, \psi_n(C) - S)$$

then we have irreversible adsorption.

To apply (1) in site, the hydrodynamical and geochemical datas included in **D**, ψ_e and ψ_n are needed. These can be determined in the solution of the corresponding inverse problems. For this purpose, precise and very efficient numerical method is needed solving the direct problem, i.e., when all model datas are known. Many of these model datas one can obtain in laboratory conditions with a column.

The main goal of this contribution is the construction of a precise and efficient numerical methods to solve 1D problems of the type (1). If an equilibrium adsorption in (1) (i.e., $\Psi_n(s) \equiv 0$) is considered with $\psi(C) = \frac{aC^p}{1+bC^p}$ and $0 \leq p < 1$, then the solution can have profile of the damped travelling wave with sharp front. Moreover, this phenomenon is strengthened when an irreversible adsorption is considered with the pulse type of initial concentration profile. The additional numerical difficulties are added when the problem is convection dominant. The numerical solution of this type of problems needs a special type of treatment.

There are many numerical methods devoted to the solution of these type of problems. Some of them using some types of “up winding”, or regularizations (see [9, 7]), operator splitting (see [2, 3]) and interface modelling (see [1]). The “up winding”, or regularizations introduce the additional numerical dispersion which dampes the sensitivity of the solution on model parameters. In [2, 3] the splitting has been applied to diffusion, convection and adsorption and semianalytical solution has been found for nonlinear convection only for the Langmuir and Freundlich isotherms. The interface modelling is a very powerful method, however, the interface evolution model is required. For nonequilibrium adsorption model in (1) nothing is known about the existence of the interface (interface is the boundary of the support of the solution).

In the present paper we construct the numerical method for (1) based on MOL (space discretization) leading to the ODE system.

In the first method, developed in [4] (see also references there) this ODE-system results by using moving grid points. The profit of this method is that the sharp fronts of the solution are captured by automatic adaptivity of moving grid points and the corresponding ODE-solver needs not to be restarted along the time evolution. This will be presented in Section 1.

In the second method we solve this system using fixed grid and operator splitting, where the splitting between adsorption phenomenon on one hand and

convection-diffusion phenomenon on other hand is applied. The reason is that the time scaling for adsorption and convection-diffusion is different at least one order which leads to very stiff ODE system. The profit of this strategy is twofold. The solution of adsorption part leads to a single ODE in each (space) grid point. On every time section we can redistribute the density of grid points which suits to the solution profile. The disadvantage of this splitting is that at every time section we have to restart the ODE-solver.

We consider the 1D case of (1) with $x \in (0, t)$, $t > 0$ and for simplicity we assume $\mathbf{v} = V \equiv \text{const}$, $\mathbf{D} \equiv \text{const} = D$, $\theta = 1$ and denote by $F(C) := C + \rho\Psi_e(C)$ in (1).

Together with (1) we consider (in 1D) the initial and boundary conditions

$$C(x, 0) \equiv 0, S(x, 0) \equiv 0; \quad C(0, t) = C0, C(L, t) = 0. \quad (2) \quad \boxed{\text{IBC}}$$

We shall use the value $C0 = 1$, which can switch at a prescribed time to the value $C0 = 0$. The more general boundary conditions for C can be considered, too. To discuss the efficiency of the numerical approximation it is sufficient to consider the progress of the input from the boundary $x = 0$ up to $x = L$. Let us consider a space discretization with the moving grid points

$$0 = x_0 < x_1(t) < \dots < x_i(t) < \dots x_N = L$$

which are not yet determined. Consider the solution $C(x_i(t), t)$ along the curve $(x_i(t), t)$. Then we rewrite (1) in the form (Lagrange coordinates)

$$\begin{aligned} \partial_t F(C(x_i(t), t)) &= F'(C(x_i(t), t))[\dot{x}_i(t)\partial_x C(x_i(t), t) + \partial_t C(x_i(t), t)] = \\ &-V\partial_x C(x_i(t), t) + D\partial_x^2 C(x_i(t), t) - \rho\kappa(\Psi_n(C(x_i(t), t)) - S), \quad (3) \quad \boxed{\text{e2:1}} \\ \partial S(x_i(t), t) + \dot{x}_i(t)\partial_x S(x_i(t), t) &= \kappa(\Psi_n(C(x_i(t), t)) - S). \end{aligned}$$

We apply here the space discretization and denote by $y_i(t)$ an approximation of $C(x_i(t), t)$ and by $w_i(t)$ an approximation of $S(x_i(t), t)$. To approximate $\partial_x C$, $\partial_x^2 C$ and $\partial_x S$ at the grid point x_i we use the three point approximation using the Lagrange polynomial of the second order crossing the points

$$(x_{i-1}(t), y_{i-1}(t)), (x_i(t), y_i(t)), (x_{i+1}(t), y_{i+1}(t))).$$

Then $y(t) := (y_1(t), \dots, y_{N-1})$ and $w(t) := (w_0(t), w_1(t), \dots, w_{N-1}(t))$ representing the numerical approximation of (1), (2), we determine by an ODE-system. For the determination of $x(t) := (x_1(t), \dots, x_{N-1}(t))$ we follow the [4] where the density of moving grid points automatically follows the high spacial activity of the solution. For this purpose it is defined the monitoring function

$$m \equiv m(x; C, S) := \sqrt{\gamma + \frac{1}{2}(\partial_x C)^2 + \frac{1}{2}(\partial_x S)^2}, \quad \text{with } \gamma > 0.$$

In the place of C, S we take their approximations y, w and use the central difference for the space derivative.

Denote by $\alpha_i(t) := x_i(t) - x_{i-1}(t)$ for $i = 1, \dots, N$ with $\alpha_0 = 0$. Then $n_i := \frac{1}{\alpha_i}$, $i = 1, \dots, N$ represent the densities of grid points. The mathematical model for moving grids is based on the following two criteria:

$$\frac{k}{k+1} \leq \frac{n_{i-1}}{n_i} \leq \frac{k+1}{k}. \quad (4) \quad \boxed{\text{eq5.1}}$$

and

$$\frac{n_{i-1}}{m_{i-1}} = \frac{n_i}{m_i}, \quad i = 2, \dots, N-1. \quad (5) \quad \boxed{\text{eq6.1}}$$

Efficiency of this numerical modelling is demonstrated on a series of numerical experiments.

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