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CONTAMINANT TRANSPORT WITH ADSORPTION IN DUAL-WELL FLOW*

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Abstract. Numerical approximation schemes are discussed for the solution of contaminant transport with adsorption in dual-well flow. The method is based on time stepping and operator splitting for the transport with adsorption and diffusion. The nonlinear transport is solved by Godunov's method. The nonlinear diffusion is solved by a finite volume method and by Newton's type of linearization. The efficiency of the method is discussed.

Keywords: nonlinear transport, operator splitting, transport of contaminants, dual-well flow

MSC 2000: 30C20, 65M25, 76M20, 76S05

1. Introduction

Contaminant transport with adsorption is a very dynamical and difficult research area. Precise mathematical models are available and significant efforts have been done to develop efficient numerical methods for the solution. However, the solution of strongly nonlinear convection-diffusion problems with dominant convection is still an open problem. In some special cases results have been obtained. Also in our model setting a contribution towards a precise numerical solution can be obtained. For the practical implementation, realistic model data are crucial. They can be obtained by calibration of the model in situ by means of additional measurements. The determination of the required real data is then an inverse problem which is, as is well-known, an ill-posed problem. This, in turn, requires a very precise numerical solution of the direct problem (with known data). Usually, the model is calibrated by means of dual-well tests in the field. If the Dupuit-Forchheimer approximation can be used (i.e. when the vertical flow is negligible), then the steady state flow

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between the injection and extraction well can be described in a relative simple way. Then, injecting a tracer in the injection well and measuring the response in the extraction well provides additional information from which we can derive desirable hydrological and geophysical data. Single-well and double-well test techniques, based on measurements of the withdrawal breakthrough curves have been discussed in [9], [13], [14], [16], [17], [18].

Our main aim is to develop very precise numerical tools for computing contaminant transport with adsorption in dual-well tests. This contribution is a direct continuation of our results in [3] and [7].

An outline of our paper is as follows. In Section 2 we present the mathematical models and the steady-state solution of the flow problem. In Section 3 we transform the problem to bipolar coordinates and present the operator splitting. In Section 4 we give the method of solution for both the nonlinear transport and the nonlinear diffusion. In Section 5 we offer some conclusions.

2. Mathematical model

The steady state flow under the Dupuit-Forchheimer approximation can be described by the flow potential Φ (see [10]) satisfying

$$\Delta\Phi = 0 \text{ in } \Omega = \mathbb{R}^2 \setminus B_{r_1}(-d,0) \cup B_{r_2}(d,0) \tag{1}$$

with a boundary condition

$$\Phi = \Phi_1 \text{ on } \partial B_{r_1}(-d,0) \quad \text{and} \quad \Phi = \Phi_2 \text{ on } \partial B_{r_2}(d,0).$$

Here r_1 and r_2 are the radii of the extraction and the injection well centered at the points $(-d,0)$ and $(d,0)$, respectively. The height of the aquifer is denoted by H and the head h (measured from the bottom of the aquifer) relates to the potential in the following way (see [10]):

$$\begin{aligned} \Phi(x,y) &= khH - (1/2)kH^2, && \text{if } \Phi(x,y) > (1/2)kH^2 \text{ (the confined zone)},\\ \Phi(x,y) &= (1/2)kh^2, && \text{if } \Phi(x,y) < (1/2)kH^2 \text{ (the unconfined zone)}. \end{aligned}$$

Here k denotes the hydraulic conductivity. The curve $h(x,y) = H$ separates the confined and unconfined zones. The corresponding velocity field $\vec{v}$ is

$$\vec{v} = -\frac{1}{h_{\text{eff}}\theta_0}\nabla\Phi, \tag{2}$$

where θ_0 is the porosity and $h_{\text{eff}} = \min\{h, H\}$.

The transport equation for the concentration C of the contaminant/tracer, including dispersivity of the porous media and adsorption, has the form (see [1], [23])

$$h_{\text{eff}}\partial_t C = \operatorname{div}(Dh_{\text{eff}}\nabla C) - \operatorname{div}(h_{\text{eff}}\vec{v}C) - \frac{h_{\text{eff}}}{\theta_0}\varrho\partial_t S, \tag{3}$$

where D is the dispersivity tensor

$$D_{ij} = \{(D_0 + \alpha_T|v|)\delta_{ij} + \frac{v_i v_j}{|v|}(\alpha_L - \alpha_T)\}. \tag{4}$$

Here D_0 is the molecular diffusion and δ_{ij} is the Kronecker symbol. The source term is generated by adsorption in the equilibrium mode, where $S = \Psi(C)$, ϱ is the density of the porous media and $\Psi(s)$ represents the adsorption isotherm. The most common isotherms are $S = \Psi(s) = K_0 s^p$ (Freundlich isotherm) and $S = \Psi(s) = \frac{K_1 s}{1+K_2 s}$ (Langmuir), where K_0, K_1, K_2, p are model parameters which have to be calibrated. Together with (3) we consider the boundary conditions

$$C(x,t) = C_0(t) \text{ for } x \in \partial B_{r_2}, \quad \partial_\nu C(x,t) = 0 \text{ for } x \in \partial B_{r_1}, \ t > 0 \tag{5}$$

and the initial condition

$$C(x,0) = 0 \quad \text{in } \Omega.$$

3. Method of solution

Due to the symmetry with respect to the x-axis, we solve (2) in the upper half-plane, with Dirichlet conditions on the half-circles and a homogeneous Neumann condition on the parts of the x-axis bordering the domain (because of symmetry). This problem can be solved efficiently using a conformal mapping and, especially, a bipolar transformation which transforms the upper half part of Ω into a rectangle $\tilde{\Omega} = (0,\pi) \times \left(v^{(1)}, v^{(2)}\right)$, see [3] and Figs. 1–2.

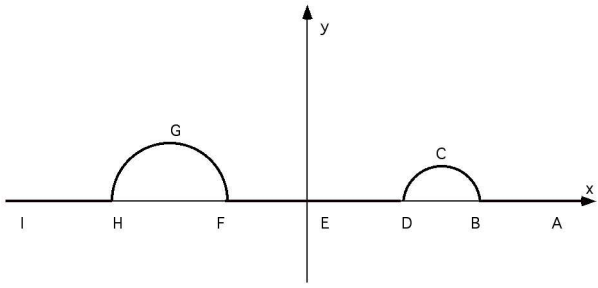

Figure 1. Boundary of the domain Ω in the (x,y) domain.

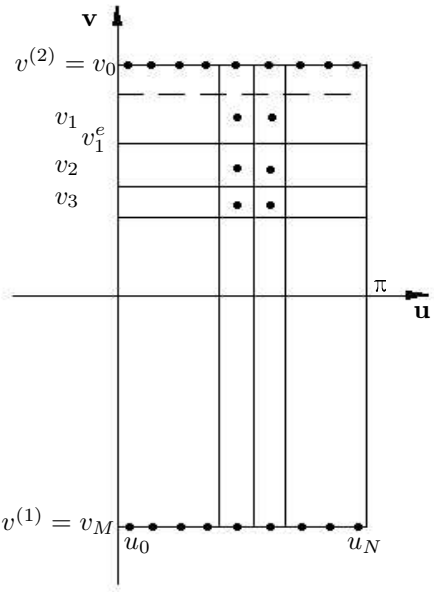

Figure 2. Boundary of the domain $\widetilde{\Omega}$ in the (u, v) domain.

Here the equipotential curves of Φ in Ω give rise to the horizontal lines in $\tilde{\Omega}$ (parallel with the u-axis). The streamlines, which are orthogonal to them, are transformed into vertical lines parallel with the v-axis. Then $\tilde{\Phi}(u, v) = \Phi(x, y)$ depends only on the v-variable and, moreover, $\tilde{\Phi}(v) = Av + B$, where A and B are to be determined from the boundary conditions. The bipolar coordinates (u, v) are defined by

$$x = \frac{\delta}{2} \frac{\sinh v}{\cosh v - \cos u}, \quad y = \frac{\delta}{2} \frac{\sin u}{\cosh v - \cos u}, \tag{6}$$

where δ can be determined from the equation

$$\sqrt{r_1^2 + \frac{1}{4}\delta^2} + \sqrt{r_2^2 + \frac{1}{4}\delta^2} = 2d \tag{7}$$

(note that $2d > r_1 + r_2$ since otherwise the wells would fail to be disjoint). As to the values $v^{(1)}$ and $v^{(2)}$, they are obtained from

$$\sinh v^{(1)} = -\frac{\delta}{2r_1}, \quad \sinh v^{(2)} = \frac{\delta}{2r_2}. \tag{8}$$

The coefficients A and B are obtained from the boundary equations

$$Av^{(1)} + B = \Phi_1, \quad Av^{(2)} + B = \Phi_2. \tag{9}$$

In this way we arrive at a simple exact solution of the flow problem in the domain $\tilde{\Omega}$ and, by the inverse transformation, in Ω.

The crucial step is to transform the transport equation (3) using the same transformation as for the potential. This was done in [3]. In our model with adsorption we obtain

$$\partial_t F(C) = g\{\partial_u(a\partial_u C) + \partial_v(b\partial_v C)\} + G\partial_v C, \tag{10}$$

where

$$F(C) = C + \frac{\varrho}{\theta_0}\Psi(C)$$

and g, a, b and G are known functions depending on u and v:

$$g = \frac{4\lambda^2}{\delta^3\theta_0 h_{\mathrm{eff}}(v)}, \quad \lambda = \cosh v - \cos u, \quad a = D_0\delta\theta_0 h_{\mathrm{eff(v)}}(v) + 2\alpha_T\lambda A,$$
$$b = D_0\delta\theta_0 h_{\mathrm{eff}}(v) + 2\alpha_L\lambda A, \quad G = \frac{4\lambda^2}{\delta^2\theta_0 h_{\mathrm{eff}}(v)}.$$

We consider boundary conditions

$$C = C_0(t) \text{ on } \Gamma_1; \quad \partial_u C = 0 \text{ on } \Gamma_2 \cup \Gamma_4; \ \partial_v C = 0 \text{ on } \Gamma_3, \tag{11}$$

where $\Gamma_1 := (0,\pi) \times \{v = v^{(2)}\}$, $\Gamma_2 := \{0\} \times (v^{(1)}, v^{(2)})$, $\Gamma_3 := (0,\pi) \times \{v^{(1)}\}$ and $\Gamma_4 := \{\pi\} \times (v^{(1)}, v^{(2)})$, together with the homogeneous initial condition

$$C((u,v),0) = 0. \tag{12}$$

The function $C_0(t)$ is the prescribed concentration at the inflow which we assume to be a constant ($C_0(t) = C^0$) or a pulse shape.

Since the convective term in (10) is only in the v-direction, one could expect that an "up wind" type of approximation (e.g. power law) would be appropriate. The results in [3] show that this introduces numerical dispersion which is larger than the one produced by dispersivity for small α_L, α_T. Therefore, we must follow a different strategy for numerical approximation.

4. Numerical approximation of (10)

To solve the above convection diffusion problem we use time stepping and operator splitting in which, for any small time interval, the problem is split into 2 parts: *the transport problem* and *the diffusion problem*. More in detail, let $\tau = T/L$, $(L \in \mathbb{N})$, be a time step and let $C_n \approx C((u,v),t_n)$ for $n = 1,\dots,L$. If C^{n-1} is known, then the relation

$$C^n = D^n(\tau)T^n(\tau)C^{n-1}, \quad \tau = t_n - t_{n-1},$$

determines C^n. The transport $T^n(\tau)$ corresponds to the solution φ of the transport equation

$$\partial_t F(\varphi) - G(u,v)\partial_v \varphi = 0, \tag{13}$$

with the inflow condition

$$\varphi\big((u,v^{(2)}),t\big) = C_0(t)$$

and the initial condition

$$\varphi((u,v),t_{n-1}) = C^{n-1}.$$

Then we put

$$C^{n,1/2} := T^n(\tau)C_{n-1} \equiv \varphi((u,v),t_n).$$

The diffusion $D^n(\tau)$ is obtained by solving the diffusion equation

$$\partial_t F(\varphi) = g\{\partial_u(a\partial_u\varphi) + \partial_v(b\partial_v\varphi)\} \tag{14}$$

with the initial condition

$$\varphi((u,v),t_{n-1}) = C^{n,1/2}.$$

Then we set

$$C^n = D^n(\tau)C^{n,1/2} = D^n(\tau)T^n(\tau)C^{n-1} \equiv \varphi((u,v),t_n).$$

The convergence analysis of the used approximation is based on convergence results for operator splitting approximation, see, e.g., [8] and [15].

The space discretization is based on the vertex-centered finite volume concept. Let $\{u_i\}_{i=0}^N$, $\{v_j\}_{j=0}^M$ be nodal points following from a not necessarily equidistant partitioning in the u- and v-direction, respectively. We generally take a non-equidistant v-partitioning following from an equidistant x-partitioning along the x-axis between the two wells. At the points $\{u_i, v_j\}$ for $j = 0$ the Dirichlet conditions for the inflow concentration C are prescribed. We have $v_0 = v^{(2)}$, $v_M = v^{(1)}$, so $v_0 > v_M$ and

$0 < u_0 < u_N < \pi$. Let $\{u_i, v_j\}$ be an inner point in $\tilde{\Omega}$. We define $\Delta u_+ = u_{i+1} - u_i$, $\Delta u_- = u_i - u_{i-1}$, $u_{i+1/2} = u_i + \Delta u_+/2$, $u_{i-1/2} = u_i - \Delta u_-/2$, $\Delta u = u_{i+1/2} - u_{i-1/2}$. We proceed analogously for v, where, e.g., $\Delta v_+ = v_{j-1} - v_j$. In this way we get u_i-strips defined by $(u_{i-1/2}, u_{i+1/2}) \times \left(v^{(1)}, v^{(2)}\right)$. In these strips we have the finite volume $V_{ij} = (u_{i-1/2}, u_{i+1/2}) \times (v_{j+1/2}, v_{j-1/2})$ corresponding to (u_i, v_j). For the edges of $\widetilde{\Omega}$ we set $u_{-1/2} \equiv 0$, $u_{N+1/2} \equiv \pi$, $v_{-1/2} \equiv v_0$ and $v_{M+1/2} \equiv v_M$.

4.1 Solution of the nonlinear transport problem.

We consider (13) in the strip $(u_{i_0-1/2}, u_{i_0+1/2}) \times \left(v^{(1)}, v^{(2)}\right)$ with shocks on the edges $v_0^e \equiv v^{(2)}$, $v_1^e \equiv v_{3/2}$, $v_2^e \equiv v_{5/2}$, …, $v_{M-1}^e \equiv v_{M-1/2}$, $v_M^e \equiv v^{(1)}$ of the finite volumes. The resulting 1D-problem can be solved by a semi-analytical method without a time step limitation for the case of Langmuir or Freundlich type isotherms—see [7]. The solution of (13) for $F(\varphi) \equiv \varphi$ has been considered in [3]. In the case of general isotherms Godunov's method can be applied for solving (13), since Godunov's flux can be determined by solving a multiple Riemann problem. Now a time step limitation will be necessary, since the general form of rarefactions cannot be obtained. The solution of the transport problem (13) will be based on a piecewise constant initial profile $\varphi_0(v)$, i.e., on the solution of the multiple Riemann problem.

In the general case of isotherms we transform (13) by using the new variable $y = y(v)$ where

$$y = G_i(v) \equiv G(u_i, v) = \int_{v^{(1)}}^{v} \frac{h_{\text{eff}}\, \mathrm{d}v}{K\lambda^2}, \quad \lambda^2 = (\cosh(v) - p_i)^2, \quad p_i = \cos u_i,$$
$$\overline{\varphi}(u_i, y) = \varphi(u_i, v) \quad i = 1, \ldots, N.$$

We obtain (index i is omitted)

$$\partial_t F(\overline{\varphi}) - \partial_y \overline{\varphi} = 0, \quad \overline{\varphi}(y, 0) = \varphi_0(v). \tag{15}$$

We apply Godunov's method to this problem. Let k be the time step $0 < k \leqslant \tau$ and h the space step discretization parameter. We denote by $\overline{\varphi}_r^l$ an approximation of $\overline{\varphi}$ at $y = hr$, $t = t_{n-1} + kl$, $l = 1, \ldots, q$. Then the approximation scheme reads

$$F(\overline{\varphi}_r^{l+1}) = F(\overline{\varphi}_r^l) + \frac{h}{k}\left[\varphi^*(F(\overline{\varphi}_r^l), F(\overline{\varphi}_{r+1}^l)) - \varphi^*(F(\overline{\varphi}_{r-1}^l), (F(\overline{\varphi}_r^l))\right] \tag{16}$$

where φ^* is Godunov's flux, which can be determined—see ([4], (13.24))—by

$$\varphi^*(F(\overline{\varphi}_r^l), F(\overline{\varphi}_{r+1}^l)) = \begin{cases} \max\limits_{F(\overline{\varphi}_r^l) \leqslant F(s) \leqslant F(\overline{\varphi}_{r+1}^l)} s, & \text{if } F(\overline{\varphi}_r^l) \leqslant F(\overline{\varphi}_{r+1}^l) \\ \min\limits_{F(\overline{\varphi}_{r+1}^l) \leqslant F(s) \leqslant F(\overline{\varphi}_r^l)} s, & \text{if } F(\overline{\varphi}_{r+1}^l \leqslant F(\overline{\varphi}_r^l). \end{cases} \tag{17}$$

The time step $k \leqslant \tau$ has to be determined in such a way that the shocks or rarefactions from the neighbouring grid points y_{l-1} and y_{l+1} do not reach y_l during the time step k, uniformly for all grid points. This leads to the condition

$$k \leqslant h \max_{1 \leqslant r \leqslant M} \frac{1}{F'(\overline{\varphi}_r^n)}. \tag{18}$$

We take the time step k such that $qk = \tau$ for some integer $q \geqslant 1$.

From the solution (15) we obtain the desired solution of (13) for each strip $i = 1, \ldots, N$ using the backward transformation. In the case that $h_2 > h_1 \geqslant H$ (confined aquifer), we can express

$$G_i(v) = \big[\overline{G}(u_i, v) - \overline{G}\big(u_i, v^{(1)}\big)\big] \frac{\delta^2 \theta_0 H}{4A},$$

where

$$\overline{G}(u_i, v) = \frac{2pz - 2}{(1-p^2)(z^2 - 2pz + 1)} + \frac{2p}{(1-p^2)^{3/2}} \arctan \frac{z-p}{\sqrt{1-p^2}}$$

with

$$z = \exp v, \quad p = \cos u_i.$$

4.2. Solution of the nonlinear diffusion problem.

We apply a vertex-centered finite volume strategy for the approximation of (14)—see [19]. We assume further that the values $C_{i,j}$ and $g_{i,j} = g(u_i, v_j)$ are dominant over $V_{i,j}$. We integrate (14) over $(t_{n-1}, t_n) \times V_{i,j}$ and use integration by parts. Let us denote $C_{i,j} = C_{i,j}^n$, $C^E = C_{ij}^E = C_{i+1,j}$, $C^W = C_{ij}^W = C_{i-1,j}$, $C^N = C_{ij}^N = C_{i,j+1}$, $C^S = C_{ij}^S = C_{i,j-1}$. We put $a^E = a_{ij}^E = a_{i+1/2,j}$ and similarly we introduce a^W, a^N, a^S, b^E, b^W, b^N, b^S. We approximate $\partial_u C$, $\partial_v C$ on the boundaries of $V_{i,j}$ by finite differences using the grid points (u_i, v_j). For instance, on the edge $(u_{j+1/2}, v)$, $v \in (v_{i-1/2}, v_{i+1/2})$ we approximate $\partial_u C \approx \frac{C^E - C}{\Delta u_+}$. Then we successfully obtain our approximation scheme

$$\begin{aligned} \omega F(C_{i,j}) + \Big(a^E \frac{\Delta v}{\Delta u_+} + a^W \frac{\Delta v}{\Delta u_-} + b^N \frac{\Delta u}{\Delta v_+} + b^S \frac{\Delta u}{\Delta v_-}\Big)\tau C_{i,j} \\ = \Big[\tau \frac{\Delta v}{\Delta u_-} a^W\Big] C_{i-1,j} + \Big[\tau \frac{\Delta v}{\Delta u_+} a^E\Big] C_{i+1,j} + \Big[\tau \frac{\Delta u}{\Delta v_+} b^N\Big] C_{i,j+1} \\ + \Big[\tau \frac{\Delta u}{\Delta v_-} b^S\Big] C_{i,j-1} + \omega F(C_{i,j}^{n-1}), \end{aligned} \tag{19}$$

where $\omega = \omega_{ij} = \frac{|V_{ij}|}{g_{ij}}$.

Taking into account the boundary conditions we have to put $a^W \equiv 0$ for the points $\{u_0, v_j\}$ and $a^E \equiv 0$ for the points $\{u_N, v_j\}$, $j = 1, \ldots, N$. Moreover, for $\{u_i, v_M\}$, $i = 0, \ldots, N$, we take $b^S \equiv 0$ in (19). The nonlinear system of algebraic equations (19) is solved by Newton type iterations, starting with $C \equiv C^{n-1}$. We also can apply a relaxation method as in [5] and [6] as follows:

$$
\begin{aligned}
(20)\quad & \omega\lambda_{l-1}\big(C_{i,j}^{(l)} - C_{i,j}^{n-1}\big) + \Big(a^E\frac{\Delta v}{\Delta u_+} + a^W\frac{\Delta v}{\Delta u_-} + b^N\frac{\Delta u}{\Delta v_+} + b^S\frac{\Delta u}{\Delta v_-}\Big)\tau C_{i,j} \\
&= \Big[\tau\frac{\Delta v}{\Delta u_-}a^W\Big]C_{i-1,j} + \Big[\tau\frac{\Delta v}{\Delta u_+}a^E\Big]C_{i+1,j} \\
&\quad + \Big[\tau\frac{\Delta u}{\Delta v_+}b^N\Big]C_{i,j+1} + \Big[\tau\frac{\Delta u}{\Delta v_-}b^S\Big]C_{i,j-1},
\end{aligned}
$$

where l is an iteration parameter and

$$
\lambda_l := \frac{F\big(C_{i,j}^{(l)}\big) - F\big(C_{i,j}^{n-1}\big)}{C_{i,j}^{(l)} - C_{i,j}}, \quad \lambda_0 := F'(C_{i,j}^{n-1})
$$

is a relaxation function. If $|\lambda_{l_0} - \lambda_{l_0-1}| < \tau$, then we stop the iterations and put $C_{i,j} := C_{i,j}^{(l_0)}$.

If $\alpha_T = 0$ and $D_0 = 0$, the diffusion is reduced only to the v-direction ($a(u, v) = 0$). Then a simple TDMA (tridiagonal matrix algorithm, see [19]) can be used to solve in each strip the one-dimensional diffusion problem.

5. Conclusion

Numerical modelling for the transport with diffusion and adsorption in injection-extraction well devices has been presented. The main purpose is to develop a precise numerical solver which can be used for model parameter identification. The parameters to be identified belong to flow and diffusion (hydraulic permeability, longitudinal and transversal dispersivity), parts of the contaminant transport and to the adsorption (adsorption isotherms). The porous media is assumed to be homogeneous. The Dupuit-Forchheimer approximation is used for the steady-state flow generated by the injection and extraction wells. On the other hand, the flow is assumed to be unconfined-confined.

The efficient numerical approximation enables us to obtain precise solutions for long time periods. Consequently, this can be successfully applied in a series of experiments for direct and inverse problems.

Some numerical experiments have been realized in [3] and [7]. As an illustrative example we present the solution of the contaminant transport problem without

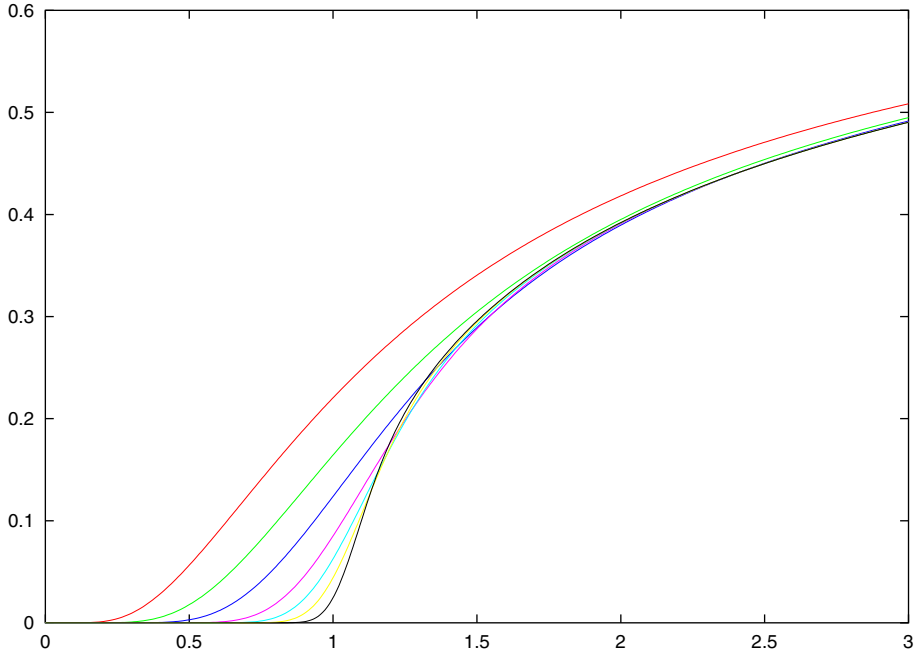

Figure 3. BTC-1 for $\alpha_L/2d = 0.2, 0.1, 0.05, 0.02, 0.01, 0.005, 0.002$ m.

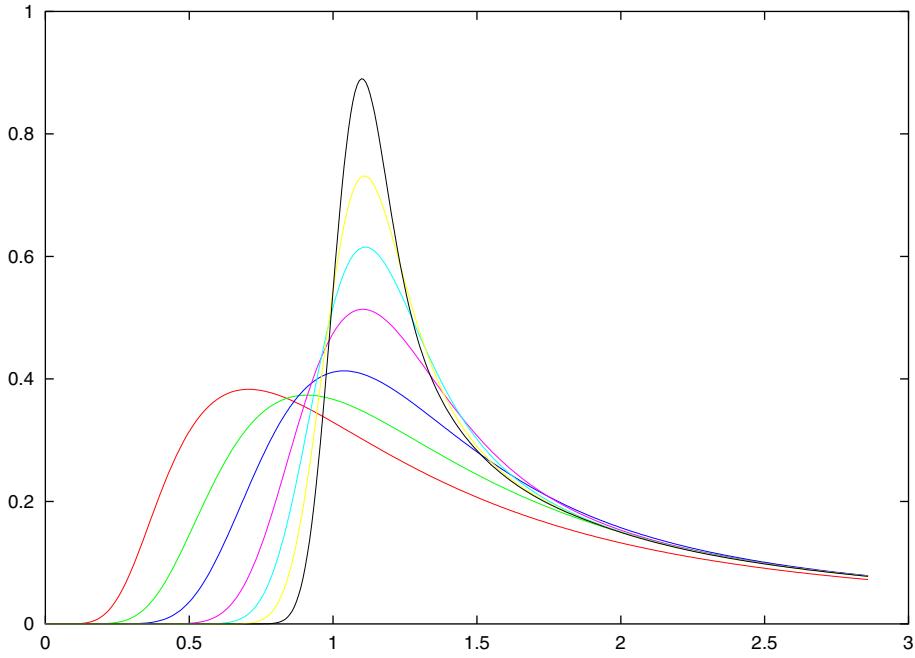

Figure 4. BTC-2 for $\alpha_L/2d = 0.2, 0.1, 0.05, 0.02, 0.01, 0.005, 0.002$ m.

adsorption from [3]. Here we demonstrate the dependence of the solution on the dispersion coefficient $\alpha_L/2d$. We shall consider two different injection regimes. In the first case we have a constant injection of the tracer, while in the second the injection is of pulse type, which lasts one day. In the numerical implementation we have used the following data: $H = 10\,\mathrm{m}$, $k = 10^{-5}\,\mathrm{m/s} = 0.864\,\mathrm{m/day}$, $r_1 = 15\,\mathrm{cm}$, $r_2 = 15\,\mathrm{cm}$, $h_1 = 10\,\mathrm{m}$, $h_2 = 15\,\mathrm{m}$. We have used the benchmark method with a 80×200 grid and a time step of 0.05 days. The break through curve (BTC) (concentration vs. time) corresponding to the injection $C_0 = 1$ is plotted in Fig. 3. The BTC corresponding to the injection with $C_0 = 1$ for 1 day and $C_0 = 0$ afterwards is plotted in Fig. 4.

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