NUMERICAL SIMULATION OF A MODEL FOR TRANSPORT AND REACTION OF RADIONUCLIDES WITH AN EXPLICIT COUPLING METHOD BETWEEN TRANSPORT AND REACTION *

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Abstract. In the last years the interest in computer simulations of radioactive waste scenarios has increased. In this article we present numerical simulations with the software package TRAPRO. We consider a system of convection-diffusion-reaction-equations, that we coupled by their reaction terms. We present a new discretization method that improves the explicit discretization for the transport- and reaction-term. The method should replace the previous decoupled implicit method with an operator-splitting method by an explicit coupled method between transport and reaction. For analyzing the method we reduce our model to a simpler system of convection-reaction-equations. The numerical results will be compared with the exact solutions. With a test example we illustrate results of our recent research on this subject.

Key words. radionuclide transport, sorption, numerical simulations

AMS subject classifications. 76S05, 80A32, 65M60

1. Introduction. The main motivation for our research is the question of how to find a suitable disposal for radioactive waste. To answer this question we have developed a software package for testing possible scenarios. We have further developed suitable discretizations and appropriate solvers, cf. [6], [7] and [9].

The model is based on a convection-diffusion-reaction-equation with kinetic sorption, see [3] and [6] . The present numerical methods, cf. [9], are standard methods of 1st order. For the space-discretization we use barycentric finite-volume methods of 1st order, cf. [2] with an upwind scheme for the convection-term, cf. [5]. For the time-discretization we use a backward-Euler-method of 1st order. As a nonlinear solver we take a Newton-method, that uses a linear solver with a biconjugate gradient method. The biconjugate gradient method uses the multigrid method as solver. The first improvements towards higher order methods were achieved in the time-discretization. We replaced the implicit first order methods by Runge-Kutta-methods of 2nd order. For the reaction-term we use an operator-splitting-method of 1st order.
In our recent work on higher order discretization we have tried to find an exact solution for the transport-reaction-term and to solve them explicitly. We could solve the problem by an operator-splitting method or by a coupled solving of transport and reaction with finite volumes.
The development of these methods and the numerical calculations are described in this paper. Numerical experiments indicate the advantages of the new method.

In Section 2 we describe the mathematical model. In Section 3 we reduce it to a simpler model. The coupled explicit method is described in Section 4, the application to a system of 2 equations is explained in Section 5. The numerical methods are explained in Section 6. First results on the simulation of a real scenario is presented

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in Section 7. In Section 8 we finish with the conclusion and discussion of the new coupling method.

2. The mathematical model. In this section we describe the model for the transport and reaction of radionuclide pollutants in groundwater flow. Further, we derive a reduced model for our experiments.

We consider a groundwater flow in a porous media. The radioactive pollutants are transported through the porous media. The retention period in the media is called mobile phase. We assume that the concentration of the pollutants does not influence the flow. A full description of the model is given in [3] and [6]. In the full model there are four different phases in which a pollutant could be. In [8], [9] we are focussed on the calculations in the mobile phase.

The quantity of the pollutant is given by the concentration depending on time and space. We will restrict ourselves to the concentration of the mobile phase in 2 space dimensions. The concentration of the i-th nuclide in the mobile phase is denoted by u^i ($[\text{mol/m}^3]$).

The transport in the mobile phase depends on the parameters of the velocity $\mathbf{v} = (v_x, v_y)^T$ and the dispersion-diffusion-tensor $D = \phi\, d^{e(i)}\, T + |\mathbf{v}|\, (\alpha_T + (\alpha_L - \alpha_T)\mathbf{v}^T \cdot \mathbf{v}/|\mathbf{v}|)$, where $d^{e(i)}$ is the molecular diffusion for the element e, T the tortuosity and α_L , α_T are the longitudinal and transversal dispersionals, respectively.

Each nuclide i corresponds to a chemical element $e(i)$. The i-th nuclide decays at rate λ^i . The nuclide has one successor and possibly more than one predecessor in the decay chain. The predecessors are denoted by $k \in k(i)$. The porosity ϕ appears in the equation as a scaling factor between the micro- and macro-scale. The retardation-factor $R_i(\phi, u^{e(i)})$ is calculated from the isotherms, cf. [6], and could be linear or nonlinear.

The equations of the mobile phase are coupled with the reaction and given by :

$$(2.1) \qquad R_i(\phi, u^{e(i)}) \left(\partial_t u^i + \lambda^i u^i - \sum_{k \in k(i)} \lambda^k u^k \right)$$

$$+ \nabla \cdot (\mathbf{v}\, u^i - D\, \nabla\, u^i) = 0 \ , \ \ u^i \ = \ u^i(x, y, t),\ (x, y, t) \in I\!\!R^2 \times I\!\!R^+ \ ,$$

$i := 1, \ldots, m$ with m : number of nuclides .

3. Reduction of the model equation. For analyzing typical phenomena of the convection-reaction-equation we consider instead of (2.1) the simplified equation (3.1) without the diffusion-term.

Here $u^{i,0} = u^i(t^0)$ is the initial condition of a delta-impulse at time $t = 0$ and $u^{i,n} = u^i(t^n)$ the concentration at time t^n. The transport-term $\nabla \cdot (\mathbf{v}\, u^{i,n} - D\, \nabla u^{i,n})$ is simplified to the velocity $\mathbf{v} = (v, 0)^T$.

The exchange reduces to an equilibrium sorption with Henry-isotherm $K_d^{e(i)}$ and is given by a constant retardation-factor $R^i = \phi + (1 - \phi)\, \rho\, K_d^{e(i)}$. The reaction-term remains the same as in (2.1). We get the reduced system of equations :

$$(3.1) \qquad R_i \left(\partial_t u^i + \lambda^i u^i - \sum_{k \in k(i)} \lambda^k u^k \right) + v\, \partial_x u^i = 0 \ ,$$

$$u^i \ = \ u^i(x, y, t),\ (x, y, t) \in I\!\!R^2 \times I\!\!R^+ \ ,$$

$i := 1, \ldots, m$ with m : number of nuclides .

4. Explicit method for coupled transport and reaction. In this section we explain the new explicit method of discretization of the coupled system. In [9] we simplify the transport-reaction equation with the decoupled method of the operator-splitting. Now we construct a coupled explicit method based on the local mass-balance, cf. [7], and exact distribution of mass.

The idea is first to calculate exactly the sinks and sources on each dual cell (cf. [2]) for the case of no transport and then to move these sinks and sources with the transport velocity.

The following steps are necessary for coupling the transport and the reaction.
1. Solving of the reaction-term, cf. [9] .
2. Coupling the reaction- and the transport-term by calculating the integration parameter for the source- and sink-terms.

We now explain these steps in detail.
1. Solving of the reaction-term, cf. [9] and [12]

$$(4.1) \qquad \partial_t u^i = -\lambda^i u^i + \frac{R^{i-1}}{R^i}\lambda^{i-1}u^{i-1},$$

is transformed to :

$$(4.2) \qquad \partial_t a^i = -\lambda^i a^i.$$

The transformation of the concentration is as follows.
1. The transformation $a^{i,n} \stackrel{\text{def}}{=} f_1(u^{1,n}, \cdots, u^{i,n})$ is given by

$$(4.3) \qquad a^{i,n} = u^{i,n} + \sum_{k=1}^{i-1} \frac{R^k}{R^i} \prod_{l=k}^{i-1} \frac{\lambda^l}{\lambda^l - \lambda^i} u^{k,n}.$$

2. The i-th equation in (4.2) has the solution

$$(4.4) \qquad a^{i,n+1} = a^{i,n}\, e^{-\lambda^i \tau^n}.$$

3. This solution is re-transformed by $u^{i,n+1} \stackrel{\text{def}}{=} f_2(a^{i,n+1}, u^{1,n+1}, \cdots, u^{i-1,n+1})$:

$$(4.5) \qquad u^{i,n+1} = a^{i,n+1} - \sum_{k=1}^{i-1} \frac{R^k}{R^i} \prod_{l=k}^{i-1} \frac{\lambda^l}{\lambda^l - \lambda^i} u^{k,n+1}.$$

4. This solution is prepared for the integration of the sink- and source-terms

$$u^{i,n+1} = u^{i,n}\, e^{-\lambda_i \tau^n}$$

$$+ \left(\sum_{k=1}^{i-1} \frac{R^k}{R^i} \prod_{l=k}^{i-1} \frac{\lambda^l}{\lambda^l - \lambda^i} u^{k,n} \right) e^{-\lambda_i \tau^n} - \sum_{k=1}^{i-1} \frac{R^k}{R^i} \prod_{l=k}^{i-1} \frac{\lambda^l}{\lambda^l - \lambda^i} u^{k,n+1}$$

$$(4.6) \qquad u^{i,n+1} \stackrel{\text{def}}{=} u^{i,n}\, e^{-\lambda_i \tau^n} + f_3(u^{1,n}, \cdots, u^{i-1,n}) .$$

Therefore the sink in the function $u^{i,n+1}$ is $u^{i,n}\, e^{-\lambda_i \tau^n}$ and the source-term with the coupled concentration is $f_3(u^{1,n}, \cdots, u^{i-1,n})$.

2. Coupling with the transport-term :

The main idea is that the mass-conservation is given by

$$(4.7) \qquad \sum_{i=1}^{m} \sum_{j=1}^{I} m_j^{i,n} = \sum_{i=1}^{m} \sum_{j=1}^{I} m_j^{i,n+1} ,$$

for any time-interval $(t^n, t^{n+1}) \subset (0, T)$, $n = 0, 1, \dots$ and for the computational cells $\Omega_j \subset \Omega$, $j = 1, \dots, I$, for the equations $i = 1, \dots, m$.

We distinguish the source- and sink-terms in (4.6).

For the computation of the source term on a cell, all predecessor cells have to be taken into account. In contrast, the sink terms we computed on each cell separately.

The idea is to find the fraction of mass that remains in cells j and $j + 1$. The source term affected by velocities on the predecessor cells which are used to calculate the fraction of mass in the cells j and $j + 1$. To calculate the affected areas in the cells we get the minima area $v_{min} \ \tau^n$ and maxima area $v_{max} \ \tau^n$ in the cells.

The set of indices $k(i)$ denotes the predecessors of the element i. To get the velocity of the equation we divide by the retardation-factors R_i and get $v_i = \frac{v}{R_i}$. To get the minimal and maximal velocity in the dual cell we calculate

$$v_{min_i} = \min_{l \in k(i)} \{ v_i, v_l \} ,$$
$$(4.8) \qquad v_{max_i} = \max_{l \in k(i)} \{ v_i, v_l \} .$$

We consider the transport in 1 dimension from the dual cell j to the cell $j + 1$. The coupling between transport and reaction is given for the dual cells j and $j + 1$ by the following distribution :

$$(4.9) \qquad t \in \left(0, \frac{x - v_{min_i} \tau^n}{v_{max_i} - v_{min_i}} \right) \quad \text{for} \quad j ,$$

$$(4.10) \qquad t \in \left(\frac{x - v_{min_i} \tau^n}{v_{max_i} - v_{min_i}}, \tau^n \right) \quad \text{for} \quad j + 1 .$$

The integration-parameter over the area in the dual cell j and $j + 1$ is given by

$$(4.11) \qquad x \in (0, v_{min_i} \tau^n), (v_{min_i} \tau^n, v_{max_i} \tau^n), (v_{max_i} \tau^n, h) \ \text{for} \ j \text{ and } j + 1 .$$

Now we consider the sink and source terms in equation (4.6). For the calculation of the sink term the velocity is taken into account. The source term is calculated using the minimum and maximum velocity of the affected equations, cf. (4.8).

$$(4.12) \qquad m_j^{i,n+1} = u_j^{i,n} e^{-\lambda_i \tau^n} (h - v_i \tau^n)$$

$$+ \int_{v_{min_i} \tau^n}^{v_{max_i} \tau^n} f_3(u_j^{1,n}, \dots, u_j^{i-1,n})\Big|_0^{\frac{x - v_{min_i} \tau^n}{v_{max_i} - v_{min_i}}} dx$$

$$+ \int_{v_{max_i} \tau^n}^{h} f_3(u_j^{1,n}, \dots, u_j^{i-1,n})\Big|_0^{\tau^n} dx .$$

$$(4.13) \qquad m_{j+1}^{i,n} = u_j^{i,n} e^{-\lambda_i \tau^n} v_i \tau^n$$

$$+ \int_0^{v_{min_i} \tau^n} f_3(u_j^{1,n}, \dots, u_j^{i-1,n})\Big|_0^{\tau^n} dx$$

$$+ \int_{v_{min_i} \tau^n}^{v_{max_i} \tau^n} f_3(u_j^{1,n}, \dots, u_j^{i-1,n})\Big|_{\frac{x - v_{min_i} \tau^n}{v_{max_i} - v_{min_i}}}^{\tau^n} dx .$$

To check the exact mass balance for the equation (4.12), we compare the sum of the two masses given in (4.12) with the mass given before mass transport.
We get the exact mass balance by :
$$m_j^{i,n+1} + m_{j+1}^{i,n+1} = u_j^{i,n} \, e^{-\lambda_i \, \tau^n} \, h + f_3(u_j^{1,n}, \ldots, u_j^{i-1,n}) \, h.$$

5. Application of the new method to a system of 2 equations. We consider the following equations :

$$\frac{\partial u_1}{\partial t} + v_1 \frac{\partial u_1}{\partial x} = -\lambda_1 u_1 \, , \tag{5.1}$$

$$\frac{\partial u_2}{\partial t} + v_2 \frac{\partial u_2}{\partial x} = -\lambda_2 u_2 + \frac{R_1}{R_2} \lambda_1 u_1 \, . \tag{5.2}$$

We assume that $v_1 \neq v_2$, $\lambda_1 \neq \lambda_2$, $v_{min} = \{v_1, v_2\}$ and $v_{max} = \{v_1, v_2\}$. We set for the concentration of the cells j and $j+1$:

Sink :

$$u_j^{2,n+1} = u_j^{2,n} \, e^{-\lambda_2 \, \tau^n} \quad \text{for } x \in (v_2 \, \tau^n, h) \, , \tag{5.3}$$

$$u_{j+1}^{2,n+1} = u_j^{2,n} \, e^{-\lambda_2 \, \tau^n} \quad \text{for } x \in (0, v_2 \, \tau^n) \, , \tag{5.4}$$

Source :

$$u_j^{2,n+1} = 0 \quad \text{for } x \in (0, v_{min} \, \tau^n) \, , \tag{5.5}$$

$$u_j^{2,n+1} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \, \left(e^{-\lambda_2 \frac{x - v_{min} \, \tau^n}{v_{max} - v_{min}}} - e^{-\lambda_1 \frac{x - v_{min} \, \tau^n}{v_{max} - v_{min}}} \right) \tag{5.6}$$
$$\text{for } x \in (v_{min} \, \tau^n, v_{max} \, \tau^n) \, ,$$

$$u_j^{2,n+1} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \, (e^{-\lambda_2 \, \tau^n} - e^{-\lambda_1 \, \tau^n}) \quad \text{for } x \in (v_{max} \, \tau^n, h) \, , \tag{5.7}$$

$$u_{j+1}^{2,n+1} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \, (e^{-\lambda_2 \, \tau^n} - e^{-\lambda_1 \, \tau^n}) \quad \text{for } x \in (0, v_{min} \, \tau^n) \, , \tag{5.8}$$

$$u_{j+1}^{2,n+1} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \, \left(e^{-\lambda_1 \frac{x - v_{min} \, \tau^n}{v_{max} - v_{min}}} - e^{-\lambda_2 \frac{x - v_{min} \, \tau^n}{v_{max} - v_{min}}} \right. \tag{5.9}$$
$$\left. + e^{-\lambda_2 \, \tau^n} - e^{-\lambda_1 \, \tau^n} \right) \quad \text{for } x \in (v_{min} \, \tau^n, v_{max} \, \tau^n) \, ,$$

$$u_{j+1}^{2,n+1} = 0 \quad \text{for } x \in (v_{max} \, \tau^n, h) \, . \tag{5.10}$$

The concentration is integrated over the intervals, cf. (4.11), and so we get the flowing equations for the masses :

Sink :

$$m_j^{2,n} = u_j^{2,n} \, e^{-\lambda_2 \tau^n} (h - v_2 \, \tau^n) \, , \tag{5.11}$$

$$m_{j+1}^{2,n} = u_j^{2,n} \, e^{-\lambda_2 \tau^n} v_2 \, \tau^n \, , \tag{5.12}$$

Source :

$$m_j^{2,n} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \, \left(\frac{v_{max} - v_{min}}{\lambda_2} (1 - e^{-\lambda_2 \tau^n}) \right. \tag{5.13}$$
$$\left. + \frac{v_{max} - v_{min}}{\lambda_1} (e^{-\lambda_1 \tau^n} - 1) + (h - v_{max} \tau^n)(e^{-\lambda_2 \tau^n} - e^{-\lambda_1 \tau^n}) \right) \, ,$$

$$(5.14) \qquad m_{j+1}^{2,n} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \left((e^{-\lambda_2 \tau^n} - e^{-\lambda_1 \tau^n}) \, v_{max} \tau^n \right.$$
$$\left. + \frac{v_{max} - v_{min}}{\lambda_1} (1 - e^{-\lambda_1 \tau^n}) + \frac{v_{max} - v_{min}}{\lambda_2} (e^{-\lambda_2 \tau^n} - 1) \right) .$$

For the two dimensional case we use the description of the flux-discretization with inflow- and outflow-notation, cf. [7].

$$(5.15) \qquad m_{jk}^{1,n} = u_j^{1,n} \, v_{jk_1} \, \tau^n e^{-\lambda_1 \tau^n} ,$$

$$(5.16) \qquad m_{jk}^{2,n} = u_j^{1,n} \, \frac{R_1}{R_2} \frac{\lambda_1}{\lambda_1 - \lambda_2} \left((e^{-\lambda_2 \tau^n} - e^{-\lambda_1 \tau^n}) \, v_{jk_{max}} \tau^n \right.$$
$$+ \frac{v_{jk_{max}} - v_{jk_{min}}}{\lambda_1} (1 - e^{-\lambda_1 \tau^n}) + \frac{v_{jk_{max}} - v_{jk_{min}}}{\lambda_2} \left. (e^{-\lambda_2 \tau^n} - 1) \right)$$
$$+ u_j^{2,n} \, v_{jk_2} \, \tau^n e^{-\lambda_2 \tau^n} .$$

Here $v_{jk} = |\Gamma_{jk}| \, (\mathbf{n} \cdot \mathbf{v})(x_{jk})$, $\mathbf{v} = (v, 0)^T$. Γ_{jk} is the line segment between the computational cells Ω_j and Ω_k. x_{jk} is the middle point of the line segment Γ_{jk}. The flow for the velocity v_i is given by $v_{jk_i} = \frac{v_{jk}}{R_i}$, for $i = 1, 2$.
The values of the minimum and the maximum retardation-factors are given by $R_{min} = \min\{R_1, R_2\}$, $R_{max} = \max\{R_1, R_2\}$. The minimum and maximum flows are given by $v_{jk_{min}} = \frac{v_{jk}}{R_{min}}$ and $v_{jk_{max}} = \frac{v_{jk}}{R_{max}}$.
The equation (5.15) is inserted in the discretization, cf. [7], so we get

$$(5.17) \qquad V_j \, u_j^{i,n+1} = V_j \, u_j^{i,n} - \sum_{k \in out(j)} m_{jk}^{i,n} + \sum_{l \in in(j)} m_{lj}^{i,n} \text{ for } i = 1, 2.$$

6. Numerical methods. The method described in Section 4 for solving equation (2.1) is implemented in the flexible software-package TRAPRO.

We have programmed a flexible input interface for reading the different model-parameters from input-files in runtime.

The program-package uses the powerful library of the software-package UG, cf. [1]. We use the efficient sparse matrix storage for our equations, cf. [10].

For the implicit discretization we use an implicit backward-Euler-method. The explicit discretization uses a modified TVD-method with a time-limiter, cf. [8] and [11] .
The implicit method uses an operator-splitting method, cf. [9], and the explicit method uses the new method described in Section 4 . Finally, we applied our method to two numerical experiments.

7. Numerical results. In the first experiment we use an initial condition at initial time $t^0 = 0.0$ and at initial area $(x^0, y^0) \in ((0.125, 0.375) \times (0.375, 0.625))$, with $u^1(x^0, y^0, t^0) = 1.0$ and $u^2(x^0, y^0, t^0) = 0.0$. The velocities are $v_1 = 0.01$ and $v_2 = 0.0$, the decay-rates are $\lambda_1 = 0.01$ and $\lambda_2 = 1.0 \, 10^{-6}$. For analyzing the transport we compute only the first time-step. We compare two different discretizations for the transport.

The results of the calculation by the operator-splitting method are shown in the first two pictures in Figure 7.1. The operator-splitting method consists of two steps, first the decay- and then the transport-step. In the first picture we see the initial concentration u^1, in the second picture the concentration u^2 after the first time-step. As $v_2 = 0.0$ the concentration u^2 is not transported in the first time step.

The analogous results of the computation with the explicit coupling method are shown in the last two pictures in Figure 7.1.

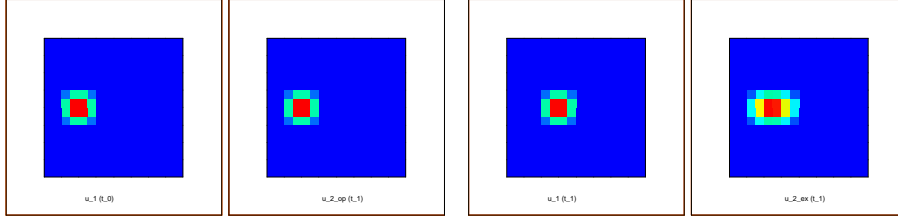Due to coupling of decay and transport, u^2 is transported already in the first time-step.

FIG. 7.1. *Calculation with Operator-Splitting and coupled Explicite Method*

The second experiment is taken from a realistic problem of radionuclide transport in porous media. The exact solution of the equations are known, cf. [6], and are compared with the numerical results.

To support the results, cf. Section 1, different test cases are computed with modified grid- and time-steps. The parameters for the equations are given by $R_1 = 50.5$, $R_2 = 1.0$, $\lambda_1 = 7.6 \ 10^{-3}$, $\lambda_2 = 2.2 \ 10^{-4}$, for the velocity and the dispersion we get $v = 0.2$, $\alpha_L = 1.0$, $\alpha_T = 0.1$ and $\phi = 0.5$.

We compare the result with in L_1-norm computed by
$$E_{L_1}^l := \sum_{i=1}^m \sum_{j=1}^I V_j \ |u_j^{i,n} \ - \ u^i(x_j, y_j, t^n)| \ .$$

Table 7.1 shows the results in the L_1-norm for different grid- and time-steps. The results with the new method are significantly better. Figure 7.2 we see the result of

The method	l	Δt	$E_{L_1}^l$	timesteps
implicit method with OP	4	0.25	$1.99 \ 10^{-2}$	10
implicit method with OP	5	0.125	$3.93 \ 10^{-3}$	20
implicit method with OP	6	0.0625	$9.866 \ 10^{-4}$	40
explicit coupling method	4	0.25	$1.25 \ 10^{-2}$	10
explicit coupling method	5	0.125	$3.39 \ 10^{-3}$	20
explicit coupling method	6	0.0625	$7.003 \ 10^{-4}$	40

TABLE 7.1
Comparison between implicit decoupling and explicit coupling method

the two equations. The different velocities are $v_1 = 0.2/50.5$ and $v_2 = 0.2/1.0$. We use a grid with 24576 elements. The timestep is $\Delta t = 0.0625$. The pictures on the left hand side in Figure 7.2 shows the initial concentrations at time $t_{100} = 100 \ a$, the pictures on the right hand side in Figure 7.2 shows the concentrations at time $t_{200} = 200 \ a$.

8. Conclusions. We have presented a new method for the numerical computation of a certain class of transport-reaction equations with different retardation-factors. We have shown, in particular, how to solve an explicit method that couples transport and reaction exactly. With our new method we are able to solve the considered systems exactly. Our current work is now focussed on kinetic sorption, with the combination with the exact explicit method.
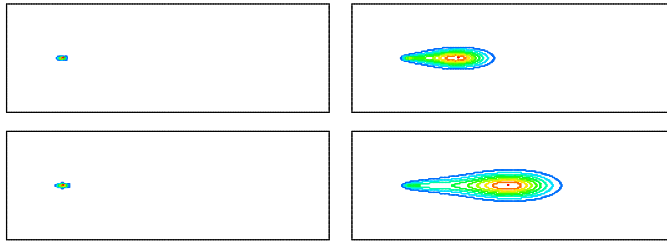
FIG. 7.2. $u^i(t^n)$ for $n = 1, 2$ at $t^1 = 100a$ (initial condition) and at $t^2 = 200a$.

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