Spatial-dependent and Nonlinear fluid transport: Coupling Framework

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Abstract. We introduce a solver method for spatial-dependent and nonlinear fluid transport. The motivation is driven by transport processes in porous medias (e.g. waste disposal, chemical deposition processes).
We analyze the coupled transport-reaction equation with mobile and immobile areas.
The main idea is to apply transformation methods to spatial and nonlinear terms to obtain linear or nonlinear ordinary differential equations. Such differential equations can simpler solved with Laplace-transformation methods or nonlinear solver methods, see [25].
The nonlinear methods are based on characteristic methods and can be generalised numerically to higher-order TVD methods, see [20].
In this article we will focus on the derivation of the analytical solutions for spatial- and nonlinear problems, that can be embedded into finite volume methods.
At the end of the article we illustrate numerical experiments for different benchmark problems.

Key words: advection-reaction equation, spatial and nonlinear transport, Laplace transformation, analytical solutions, finite volume methods.

AMS subject classifications. 35K15 35K57 47F05 65M60 65N30

1 Introduction

We study real-life problems in the direction of deposition processes given by transport and reaction models.

The modeling is based an a homogenization of the underlying media, see [3] and [4].

We deal with the following processes in the fluid transport:

- Transport, Sorption and Reaction of the mobile concentration in mobile Groundwater

– Sorption and Reaction of the immobile concentration in the immobile Groundwater

– Kinetic Sorption and Reaction in the adsorpted phase

Based on such processes the derived modeling equations are given as:

$$
\begin{aligned}
&\phi\, \partial_t\, C_i^L + \partial_t\, (g(1-\phi-\phi_{im})\rho C_i^{ad}) \\
&+\ \nabla \cdot (\boldsymbol{q}\, C_i^L - D\, \nabla\, C_i^L) \\
&= -\lambda_i(\phi C_i^L + g(1-\phi-\phi_{im})\rho C_i^{ad}) \\
&+ \sum_{k(i)} \lambda_k(\phi C_k^L + g(1-\phi-\phi_{im})\rho C_k^{ad}) \\
&- \alpha^e(i)(C_i^L - G_i^L) + \tilde{Q}_i^d - Q_f \rho_f C_i^L
\end{aligned}
\tag{1}
$$

C_L^i : i-th concentration of the mobile species
C_{ad}^i : i-th concentration of the adsorbed pollutant
G_L^i : i-th concentration solved in the immobile groundwater
λ^i : i-th decay rate $(\lambda^0 = 0.0)$
$\boldsymbol{q}$: Darcy-velocity-vector
D : Diffusive-dispersive tensor
ϕ : effective porosity
ϕ_{im} porosity of the immobile aquifer
ρ : density of the aquifer
g : factor for matrix-surface for the immobile and mobile part
$\alpha^{e(i)}$: element rate for exchange after Coat-Smith
Q_f : fluid sources or sinks
$\tilde{Q}_i$: Sources or sinks for the i-th species
ρ_f : fluid density

Formulation of the equilibrium sorption :

$$Henry - Isotherm:$$
$$C_i^{ad} = K_d^{e(i)} C_i^L \tag{2}$$

$$Langmuir - Isotherm:$$
$$C_i^{ad} = \frac{b\kappa}{1 + bC_{e(i)}^L} C_i^L \tag{3}$$

$$Freundlich - Isotherm:$$
$$C_i^{ad} = \frac{K_{nl}(C_{e(i)}^L)^p}{C_{e(i)}^L} C_i^L \tag{4}$$

$K_d^{e(i)}$: element specified K_d value for the Henry-Isotherm
b : element specified sorption-constant for the Langmuir-Isotherm
κ : element specified sorption-capacity of Langmuir
K_{nl} : element specified sorption-constant for the Freundlich-Isotherm
p : element specified exponent for the Freundlich-Isotherm

Formulation for the kinetic Sorption :

$$Henry - Isotherm:$$
$$\frac{\partial}{\partial t} C_i^{ad} = k_\alpha^{e(i)} (K_d^{e(i)} C_i^L - C_i^{ad}) \tag{5}$$
$$+ \lambda_i C_i^{ad} + \sum_{k(i)} \lambda_k C_k^{ad})$$

$$Langmuir - Isotherm:$$
$$\frac{\partial}{\partial t} C_i^{ad} = k_\alpha^{e(i)} (\frac{b\kappa}{1 + bC_{e(i)}^L} C_i^L - C_i^{ad}) \tag{6}$$
$$+ \lambda_i C_i^{ad} + \sum_{k(i)} \lambda_k C_k^{ad})$$

$$Freundlich - Isotherm:$$
$$\frac{\partial}{\partial t} C_i^{ad} = k_\alpha^{e(i)} (\frac{K_{nl}(C_{e(i)}^L)^p}{C_{e(i)}^L} C_i^L - C_i^{ad}) \tag{7}$$
$$+ \lambda_i C_i^{ad} + \sum_{k(i)} \lambda_k C_k^{ad})$$

k_α : element specified velocity-rate for the kinetic sorption

Formulation of the immobile pore-water :

$$\frac{\partial}{\partial t} \left(\phi_{im} \; G_i^L + \; (1-g)(1-\phi-\phi_{im})\rho G_i^{ad}\right) \tag{8}$$

$$= -\lambda_i(\phi_{im} G_i^L + (1-g)(1-\phi-\phi_{im})\rho G_i^{ad})$$

$$+ \sum_{k(i)} \lambda_k (\phi_{im} G_k^L + (1-g)(1-\phi-\phi_{im})\rho G_k^{ad})$$

$$+ \alpha^e(i)(C_i^L - G_i^L) \tag{9}$$

G^i_{ad} : i-th concentration solved in the immobile groundwater from the adsorbed species

1.1 Description of the physical model

The physical motivation arose to model a nonlinear fluid transport in a porous media with multiple phases.

The following processes are included to the physical model:

- Reaction and Transport of radioactive waste.
- Four different phases in which the species can be.
- Species in the Mobile phase of the groundwater are transported by the flow.
- Species in the immobile phase of the groundwater are remain at a fixed position.
- Species could be adsorbed by the matrix in a mobile adsorbed and an immobile adsorbed phase.

In figure 1, we see the different species that are located in the four phases.

Based on the important sorption processes, which are influencing nonlinear the model equations, the solutions are delicate to obtain in an analytical framework.

We concentrate on the main idea of the traveling waves, which allows to transform into ordinary differential equations. Physically, the traveling waves are paths of the moving species on which they react with other species.

The paper is organized as follows. One of the main contributions are the one-dimensional analytical solutions. The application for spatial dependent equations are described in section 2. In section 3, the construction of the nonlinear differential equations in different situations is presented. The verification of the new discretization method in various numerical examples is performed in section 4. At the end of this paper we introduce future works.

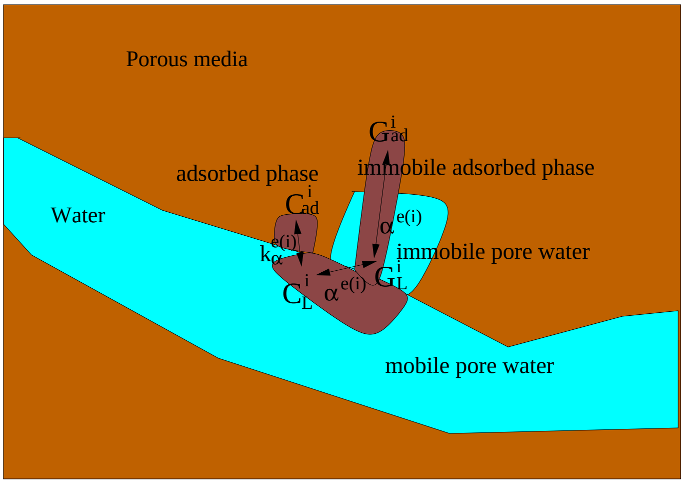

Fig. 1. Concentration in the porous media

2 Spatial dependent Case

For the spatial dependent case, we restrict us to the following equations, which are coupled with the reaction terms and are presented as follows.

$$\partial_t R_i u_i + e_i(x,t) \nabla \cdot \mathbf{v}\; u_i = -\lambda_i \; g_i(t) \; R_i \; u_i + \lambda_{i-1} \; R_{i-1} \; g_{i-1}(t) \; u_{i-1} \tag{10}$$
$$+\beta(-u_i + u_{im,i}) \;\text{ in } \Omega \times (0,T) \;,$$
$$u_{i,0}(x) = u_i(x,0) \;\text{ on } \Omega \;, \tag{11}$$
$$\partial_t R_i u_{im,i} = -\lambda_i \; R_i \; g_i(t) \; u_{im,i} \; + \lambda_{i-1} \; R_{i-1} \; g_{i-1}(t) \; u_{im,i-1} \tag{12}$$
$$+\beta(-u_{im,i} + u_i) \;\text{ in } \Omega \times (0,T) \;,$$
$$u_{im,i,0}(x) = u_{im,i}(x,0) \;\text{ on } \Omega \;, \tag{13}$$
$$i = 1, \ldots, m \;,$$

where m is the number of equations and i is the index of each component. The unknown mobile concentrations $u_i = u_i(x,t)$ are considered in $\Omega \times (0,T) \subset \mathbb{R}^n \times \mathbb{R}^+$, where n is the spatial dimension. The unknown immobile concentrations $u_{im,i} = u_{im,i}(x,t)$ are considered in $\Omega \times (0,T) \subset \mathbb{R}^n \times \mathbb{R}^+$, where n is the spatial dimension. The retardation factors R_i are constant and $R_i \geq 0$. The kinetic part is given by the factors λ_i. They are constant and $\lambda_i \geq 0$.

Further $e_i(,x,t) : \mathbb{R} \times \mathbb{R}^+ \rightarrow \mathbb{R}^+, \;\; i = 1,\ldots,m, \; f_i(t) : \mathbb{R}^+ \rightarrow \mathbb{R}^+, \;\; i = 1,\ldots,m$ are the polynomial functions of the time-dependent convection and reaction term.

For the initialization of the kinetic part, we set $\lambda_0 = 0$. The kinetic part is linear and irreversible, so the successors have only one predecessor. The initial conditions are given for each component i as constants or linear impulses. For the boundary conditions we have trivial inflow and outflow conditions with $u_i = 0$ at the inflow boundary. The transport part is given by the velocity $\mathbf{v} \in \mathbb{R}^n$ and is piecewise constant, see [13] and [14]. The exchange between the mobile and immobile part is given by β.

2.1 Analytical solutions for spatial-dependent convection equation

Scalar case We deal with the following spatial-dependent convection equation:

$$\partial_t u + e(x,t)\partial_x u = 0 \ , \ x, t \in [0, L] \times [0, T], \tag{14}$$

where we assume $e(x,t) = f(x)g(t)$ and we have polynomial functions for $f(x)$ and $g(t)$, given as $f(x) = \sum_{i=0}^{I} a_i x^i$, where $I \in \mathbb{N}_0^+$ is a given number, so for example $f(x) = (a_0 + a_1 x)$.

To solve the equation 88, we transform into a new space variable, Z by:

$$dZ = \frac{dx}{f(x)} = g(t)dt \tag{15}$$

where

$$Z = \int \frac{1}{f(x)} \, dx = \frac{\ln(f(x))}{f'(x)} \tag{16}$$

and we obtain the following equation:

$$\partial_t u + g(t)\partial_Z u = 0 \ , \ Z, t \in [Z(0), Z(X)] \times [0, T], \tag{17}$$

where $Z(x) = \frac{\ln(f(x))}{f'(x)}$ and $X \in R^+$.

This equation, we can solve the results of [17].

Example 1. We deal with

$$\partial_t u + (1 + ax)\partial_x u = 0 \ , \ x, t \in [0, X] \times [0, T], \tag{18}$$

where $a \in \mathbb{R}^+$ is a constant and $X \in \mathbb{R}^+$.
The initial condition is defined for $x \in (0, 1)$,

$$u(x, 0) = \begin{cases} b \ , \ x \in (0, 1) \\ 0 \ , \text{otherwise} \end{cases} , \tag{19}$$

where $b \in \mathbb{R}^+$ is a constant,

The transformed equation is given as:

$$\partial_t u + \partial_Z u = 0 \ , \ Z, t \in [0, Z(X)] \times [0, T], \tag{20}$$

with the initial condition:

$$u(Z, 0) = \begin{cases} b \ , \ Z \in (0, Z_0) \\ 0 \ , \quad \text{otherwise} \end{cases} , \tag{21}$$

and $Z = \frac{\ln(1+ax)}{a}$, with $Z_0 = \frac{\ln(1+aL)}{a}$, where $L = 1$.

The solution is given as,

$$u(Z(x), t) = \begin{cases} 0 \ , & Z(0) \leq Z(x) \leq Z(t) \\ b \ , & Z(t + L) \leq Z(x) \leq Z(t + L) \\ 0 \ , & Z(t + L) \leq Z(x) \end{cases} . \tag{22}$$

Vectorial case

$$\partial_t R_i u_i + e_i(x,t)\ v_i\ \partial_x u_i = -\lambda_i\ g_i(t)\ R_i\ u_i + \lambda_{i-1}\ R_{i-1}\ g_{i-1}(t)\ u_{i-1} \tag{23}$$

in $\Omega \times (0,T)$,

$$u_{i,0}(x) = u_i(x,0) \ \text{ on } \Omega\ , \tag{24}$$

$$\tag{25}$$

where m is the number of equations and i is the index of each component. The unknown mobile concentrations $u_i = u_i(x,t)$ are considered in $\Omega \times (0,T) \subset \mathbb{R}^n \times \mathbb{R}^+$, where n is the spatial dimension.

Further we assume $e_i(,x,t) = f(x) g_i(t) : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}^+,\ i = 1, \ldots, m$, $g_i(t) : \mathbb{R}^+ \to \mathbb{R}^+,\ i = 1, \ldots, m$ and $f(x)$ are the polynomial functions.

For the boundary conditions we use zero concentrations at the inflow boundary $x = 0$. The initial conditions are defined for $x \in (0,1)$,

$$\begin{aligned} u_1(x,0) &= \begin{cases} b\ , \ x \in (0,1) \\ 0\ , \text{otherwise} \end{cases}\ , \\ u_i(x,0) &= 0\ , \quad i = 2, \ldots, m\ , \end{aligned} \tag{26}$$

where b is a constant.

To solve the equation 29, we transform into a new space variable, Z by:

$$dZ = \frac{dx}{f(x)} = g_i(t) dt \tag{27}$$

where

$$Z = \int \frac{1}{f(x)}\ dx = \frac{\ln(f(x))}{f'(x)} \tag{28}$$

and we obtain the following equation:

$$\begin{aligned} &\partial_t R_i u_i + g_i(t)\ v_i\ \partial_Z\ u_i && (29) \\ &= -\lambda_i\ g_i(t)\ R_i\ u_i + \lambda_{i-1}\ R_{i-1}\ g_{i-1}(t)\ u_{i-1} \text{ in } [0, Z_0] \times (0,T)\ , \\ &u_{i,0}(Z) = u_i(Z,0) \ \text{ on } [0, Z_0]\ , && (30) \end{aligned}$$

where $Z_0 = \frac{\ln(f(L))}{f'(L)}$.

We use the Laplace transformation for the translation of the partial differential equation to the ordinary differential equation. The transformations for this case are given in [6], [18] and [21].

In equation (**??**) we apply the Laplace transformation given in [1] and [5]. For that we need to define the transformed function $\hat{u} = \hat{u}(s,t)$:

$$\hat{u}_i(s,t) := \int_0^\infty u_i(Z,t)\, e^{-sZ}\, dx\ . \tag{31}$$

From (**??**), the functions $\hat{u}_i$ satisfy the transformed equations

$$\partial_t \hat{u}_1 = -\left(\lambda_1\ g_1(t)\ + s v_1\ g_1(t)\ \right) \hat{u}_1\ , \tag{32}$$

$$\partial_t \hat{u}_i = -\left(\lambda_i\ g_i(t)\ + s v_i\ g_i(t)\ \right) \hat{u}_i + \lambda_{i-1}\ g_{i-1}(t) \hat{u}_{i-1}\ , \tag{33}$$

and the transformed initial conditions for $s \in (0, \infty)$,

$$\hat{u}_1(s,0) = \frac{b}{s}(1 - e^{-s})\,, \tag{34}$$

$$\hat{u}_i(s,0) = 0\,, \quad i = 2, \ldots, m\,.$$

Lemma 1. *We deal with the linear differential equations (48) and (33) where* $g_i : \mathbb{R} \to \mathbb{R}$, $m = 1, \ldots, m$ *are a Riemann integrable functions.*

Then the analytical solution of equations (48) and (33) are given as:

$$\begin{aligned}
\hat{u}_1(t) \; &= \hat{u}_{01} \exp(-\lambda_1 \int_0^t g_1(\tilde{t}) d\tilde{t} - s v_1 \int_0^t g_1(\tilde{t}) d\tilde{t}), && (35)\\
\hat{u}_i(t) \; &= \hat{u}_{0i} \exp(-\lambda_i \int_0^t g_i(\tilde{t}) d\tilde{t} - s v_i \int_0^t g_i(\tilde{t}) d\tilde{t}) && (36)\\
&+ \hat{u}_{0i-1} \lambda_{i-1} \; \exp(-\lambda_i \int_0^t g_i(\tilde{t}) d\tilde{t} - s v_i \int_0^t g_i(\tilde{t}) d\tilde{t}) && (37)\\
&\cdot \int_0^t \exp(\lambda_i \int_0^{s_1} g_i(\tilde{t}) d\tilde{t} + s v_i \int_0^{s_1} g_i(\tilde{t}) d\tilde{t}) \; g_{i-1}(s_1) \hat{u}_{i-1}(s_1) \; ds_1
\end{aligned}$$

where $\hat{u}(0) = (\hat{u}_{01}, \ldots, \hat{u}_{0i})^t$ *are the initial condition. We assume* i *components.*

Proof. The idea is based on the integration rule of a linear differential equation and we apply the recursive arguments.

Example 2. We obtain the analytical solution for $i = 1, 2, 3$ with $g_i : \mathbb{R} \to \mathbb{R}$:

$$\hat{u}_1(t) = \hat{u}_{01} \exp(-\lambda_1 \int_0^t f_1(\tilde{t}) d\tilde{t} - s v_1 \int_0^t g_1(\tilde{t}) d\tilde{t}), \tag{38}$$

$$\begin{aligned} \hat{u}_2(t) &= \hat{u}_{02} \exp(-\lambda_2 \int_0^t g_2(\tilde{t}) d\tilde{t} - s v_2 \int_0^t g_2(\tilde{t}) d\tilde{t}) \\ &+ \hat{u}_{01} \lambda_1 \ \exp(-\lambda_2 \int_0^t g_2(\tilde{t}) d\tilde{t} - s v_2 \int_0^t g_2(\tilde{t}) d\tilde{t}) \\ &\cdot \int_0^t \exp\left(-\lambda_1 \int_0^{s_1} g_1(\tilde{t}) d\tilde{t} - s v_1 \int_0^{s_1} g_1(\tilde{t}) d\tilde{t} + \lambda_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t} + s v_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t}\right) g_1(s_1) \ ds_1 \end{aligned} \tag{39}$$

$$\begin{aligned} \hat{u}_3(t) &= \hat{u}_{03} \exp(-\lambda_3 \int_0^t g_3(\tilde{t}) d\tilde{t} - s v_3 \int_0^t g_3(\tilde{t}) d\tilde{t}) \\ &+ \hat{u}_{02} \lambda_2 \ \exp(-\lambda_3 \int_0^t g_3(s_1) ds_1 - s v_3 \int_0^t g_3(s_1) ds_1) \\ &\cdot \int_0^t \exp\left(-\lambda_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t} - s v_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t} + \lambda_3 \int_0^{s_1} g_3(\tilde{t}) d\tilde{t} + s v_3 \int_0^{s_1} g_3(\tilde{t}) d\tilde{t}\right) g_2(s_1) \ ds_1 \\ &+ \hat{u}_{01} \lambda_1 \lambda_2 \ \exp(-\lambda_3 \int_0^t f_3(\tilde{t}) d\tilde{t} - s v_3 \int_0^t g_3(\tilde{t}) d\tilde{t}) \\ &\cdot \int_0^t \exp\left(-\lambda_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t} - s v_2 \int_0^{s_1} g_2(\tilde{t}) d\tilde{t} + \lambda_3 \int_0^{s_1} f_3(\tilde{t}) d\tilde{t} + s v_3 \int_0^{s_1} g_3(\tilde{t}) d\tilde{t}\right) \\ &\cdot \left(\int_0^{s_1} \exp\left(-\lambda_1 \int_0^{s_2} g_1(\tilde{t}) d\tilde{t} - s v_1 \int_0^{s_2} g_1(\tilde{t}) d\tilde{t} + \lambda_2 \int_0^{s_2} g_2(\tilde{t}) d\tilde{t} + s v_2 \int_0^{s_2} g_2(\tilde{t}) d\tilde{t}\right) \right. \quad (41) \\ &\left. \cdot g_1(s_2) \ ds_2 \right) g_2(s_1) \ ds_1 \end{aligned} \tag{40}$$

Remark 1. The closed forms are only possible for a helpful simplification with $f_i(t) = f(t), \forall i = 1, \ldots, m$, here we obtain an analytical integrable for of the integral in equation (36). We can use the primitive
$\int_0^t \exp(\int_0^s \lambda f(s_1) ds_1) f(s) \ ds = \frac{1}{\lambda} \exp(\int_0^s \lambda f(s_1) ds_1$ while $\lambda \in \mathbb{R}$ is a constant.
In general, the integral in equation (36) can be solved with numerical integration.

2.2 Special case

We assume $g(t) = g_i(t), \forall \ i = 1, \ldots, m$.

Based on this assumption, we can follow the linear case, see also below the proof.

We denote for further solutions:

$$\Lambda_i = \prod_{j=1}^{i-1} \lambda_j \, . \tag{42}$$

The equation (33) is solved with the solution methods for the ordinary differential equation, described in [18], and the more general case is presented in [6].

Lemma 2. *The exact solution of (48) and (33) are given as:*

$$\hat{u}_1 = \hat{u}_1(s,0)\, e^{-(\lambda_1 + s v_1)\ \int_0^t f(\tilde{t})\ d\tilde{t}} \ , \tag{43}$$

for $i = 2, \ldots, m$,

$$\hat{u}_i = \hat{u}_1(s,0)\ \Lambda_i\ \sum_{j=1}^{i} e^{-(\lambda_j + s v_j)\ \int_0^t f(\tilde{t})\ d\tilde{t}} \prod_{\substack{k=1 \\ k \neq j}}^{i} \left(s(v_k - v_j) + \lambda_k - \lambda_j\right)^{-1} \ . \tag{44}$$

Proof. The case $i = 1$ is trivial:

$$\partial_t \hat{u}_1 = -\left(\lambda_1\ g(t)\ + s v_1\ g(t)\ \right) \hat{u}_1 \ , \tag{45}$$
$$\tag{46}$$

we have to inset the solution in equation (45):

$$\hat{u}_1 = \hat{u}_1(s,0)\, e^{-(\lambda_1 + s v_1)\ \int_0^t f(\tilde{t})\ d\tilde{t}} \ , \tag{47}$$

and we obtain:

$$\partial_t \hat{u}_1 = -\left(\lambda_1\ g(t)\ + s v_1\ g(t)\ \right) \hat{u}_1 \ , \tag{48}$$
$$\tag{49}$$

which is the result.

The proof idea for $i > 1$ is given to the transformation to the linear case. see [16].

The derivation of $\hat{u}_i$ is given as:

$$\partial_t \hat{u}_i = g(t) \hat{\partial}_t u_{i,linear}, \tag{50}$$

where the linear solutions $u_{i,linear}$ can also be written with kernel $e^{-(\lambda_j + s v_j) \int_0^t f(\tilde{t})\ d\tilde{t}}$ instead of kernel $e^{-(\lambda_j + s v_j) t}$. The linear solutions are given and proofed in [16].

One can easily re-substitute the linear to the time-dependent kernel with out loosing any generality.

So we have to fulfill:

$$\partial_t \hat{u}_i = g(t) \left(-\left(\lambda_i\ + s v_i\ \right) \hat{u}_i + g(t) \lambda_{i-1} \hat{u}_{i-1}\right) \ , \tag{51}$$

and we have

$$g(t) \partial_t \hat{u}_{i,linear} = g(t) \left(-\left(\lambda_i\ + s v_i\ \right) \hat{u}_{i,linear} + g(t) \lambda_{i-1} \hat{u}_{i-1,linear}\right) \ , \tag{52}$$
$$\partial_t \hat{u}_{i,linear} = -\left(\lambda_i\ + s v_i\ \right) \hat{u}_{i,linear} + \lambda_{i-1} \hat{u}_{i-1,linear} \ , \tag{53}$$

while the linear solutions with the time-dependent kernel fulfilled the equation (53) and we are done.

The analytical solution in (44) can have a singular point for a single value of s. Nevertheless, this causes no difficulties when we apply the inverse Laplace transformation and thus we do not need to discuss this issue any further.

To obtain the exact solution of (**??**), we must apply the inverse Laplace transformation on (48). For that we have to apply some algebraic manipulations.

For the first case, let us assume that $v_j \neq v_k$ and $\lambda_j \neq \lambda_k$ for $j \neq k$ and $\forall j, k = 1, \ldots, m$. Then we can denote

$$\lambda_{kj} = \lambda_{jk} := \frac{\lambda_j - \lambda_k}{v_j - v_k} \,. \tag{54}$$

Furthermore, for the next transformation, we require that the values λ_{jk} are different for each pair of indices j and k.

The factors $\Lambda_{j,i}$ with $\lambda_j \neq \lambda_k$ for $j \neq k$ and the factor $\Lambda_{jk,i}$ with $\lambda_{jk} \neq \lambda_{jl}$ for $k \neq l$ are given by

$$\Lambda_{j,i} = \left(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_k - \lambda_j} \right) \,, \quad \Lambda_{jk,i} = \left(\prod_{\substack{l=1 \\ l \neq j \\ l \neq k}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}} \right) \,, \tag{55}$$

where we have the following assumptions:

$$1.\ v_j \neq v_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,, \tag{56}$$
$$2.\ \lambda_j \neq \lambda_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,, \tag{57}$$
$$3.\ \lambda_{jk} \neq \lambda_{jl} \ \ \forall j, k, l = 1, \ldots, m, \text{ for } j \neq k \ \wedge j \neq l \wedge k \neq l, \tag{58}$$
$$4.\ v_j \neq v_k \text{ and } \lambda_j \neq \lambda_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,. \tag{59}$$

From (55), the last term in (44) for a given index j can be rewritten in the following form,

$$\prod_{\substack{k=1 \\ k \neq j}}^{i} \left(s(v_k - v_j) + \lambda_k - \lambda_j \right)^{-1} = \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{\lambda_{jk}}{s + \lambda_{jk}} \Lambda_{jk,i} \,. \tag{60}$$

From (34), adopted in (50) and (44), the standard inverse Laplace transformation can be used and the solution u_i for (**??**) is given by

$$u_1(Z,t) \tag{61}$$
$$= \exp(-\lambda_1 \int_0^t g(\tilde{t})\, d\tilde{t}) \begin{cases} 0 \ , \ Z(0) \leq Z(x) < Z(v_1 \int_0^t g(\tilde{t})\, d\tilde{t}) \\ b \ , \ Z(v_1 \int_0^t g(\tilde{t})\, d\tilde{t}) \leq Z(x) < Z(v_1 \int_0^t g(\tilde{t})\, d\tilde{t} + L) \\ 0 \ , \ Z(v_1 \int_0^t g(\tilde{t})\, d\tilde{t} + L) \leq Z(x) \end{cases} ,$$

$$u_i(Z,t) = \Lambda_i \left(\sum_{j=1}^{i} \exp(-\lambda_j \int_0^t g(\tilde{t})\, d\tilde{t}) \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \Lambda_{jk,i} A_{jk} \right) , \tag{62}$$

$$A_{jk} = \begin{cases} 0 & , \ Z(0) \leq Z < Z(v_j \int_0^t g(\tilde{t})\, d\tilde{t}) \\ b\ (1 - \exp(-\lambda_{jk}(X(Z) - v_j \int_0^t g(\tilde{t})\, d\tilde{t}))) & , \ Z(v_j t) \leq Z < Z(v_j \int_0^t g(\tilde{t})\, d\tilde{t} + L) \\ b\ \exp(-\lambda_{jk}(X(Z) - v_j \int_0^t g(\tilde{t})\, d\tilde{t} - 1)) & \\ -b\ \exp(-\lambda_{jk}(X(Z) - v_j \int_0^t g(\tilde{t})\, d\tilde{t})) & , \ Z(v_j \int_0^t g(\tilde{t})\, d\tilde{t} + L) \leq Z \end{cases} \tag{63}$$

where the transformation is given as $Z(x) = \frac{\ln(f(x))}{f'(x)}$ and $L = 1$ and inverse transformation is given as $X(Z) = Z^{-1}(x)$.

3 Analytical solutions for nonlinear convection-reaction equations

Scalar case We deal with the following nonlinear convection-reaction equation, that are motivated of the Freundlich and Langimur Isotherms. We concentrate on the constant case of the convection part, but we could also use time- and spatial dependent functions; see the previous section:

$$\partial_t u^p + v \partial_x u = -\lambda u^p \ , \ x, t \in [0, L] \times [0, T], \tag{64}$$

where we assume $v \in \mathbb{R}^+$ and $p \in \mathbb{N}_0^+$.

$$u(x, 0) = \begin{cases} 1 \ , \ x \in (0, 1) \\ 0 \ , \ \text{otherwise} \end{cases} . \tag{65}$$

To solve the equation 64, we transform into a new variable $\tilde{c}$:

$$u(x,t) = \tilde{u}(\eta), \eta = x - vt, \tag{66}$$

where we have:

$$\frac{\partial u^p}{\partial t} = \frac{\partial \tilde{u}^p(\eta)}{\partial t} = \frac{\partial \tilde{u}^p}{\partial \eta} \frac{\partial \eta}{\partial x} = p \tilde{u}^{p-1} \tilde{u}' \ \frac{\partial \eta}{\partial t}$$
$$= p(-v) \tilde{u}^{p-1} \tilde{u}' \ , \tag{67}$$

and

$$\frac{\partial u}{\partial x} = \frac{\partial \tilde{u}(\eta)}{\partial x} = \frac{\partial \tilde{u}}{\partial \eta}\frac{\partial \eta}{\partial x}$$
$$= \tilde{u}' \tag{68}$$

and we obtain the following equation:

$$\begin{cases} -vp\ \tilde{u}^{p-1}\ \tilde{u}' + v\tilde{u}' = -\lambda \tilde{u}^p\ ,\ \ \eta = x - vt\ ,\ vt \leq x \leq vt+1 \\ 0, \qquad\qquad\qquad\qquad\qquad\qquad else \end{cases}, \tag{69}$$

where $\tilde{u}' = \frac{\partial \tilde{u}}{\partial \eta}$, and we obtain:

$$\begin{cases} (-vp\ \tilde{u}^{-1} + \tilde{u}^{-p})\partial\tilde{u} = -\lambda\partial\eta\ ,\ \ \eta = x - vt\ ,\ vt \leq x \leq vt+1 \\ 0, \qquad\qquad\qquad\qquad\qquad\qquad else \end{cases}, \tag{70}$$

and we obtain:

$$\begin{cases} -vp\ln(\tilde{u}) - p\tilde{u}^{-p-1} = -\lambda\eta + C_0(x)\ ,\ \ \eta = x - vt\ ,\ vt \leq x \leq vt+1 \\ 0, \qquad\qquad\qquad\qquad\qquad\qquad else \end{cases}, \tag{71}$$

with $C_0(x)$ is the constant, that can be found with the initial value of $c_0(x)$.
While the initial function is given as:

$$C_0(x) = -vp\ln(\tilde{\tilde{u}}) - p\tilde{\tilde{u}}^{-p-1} + \lambda x\ ,\ \ \ \eta = x\ ,\ 0 \leq x \leq 1, \tag{72}$$
$$0\ \ else\ . \tag{73}$$

where $\tilde{\tilde{u}} = u(x,0)$.
This equation, we can solve with fix-point solvers or Newton solvers.

Example 3. We deal with

$$\partial_t u^p + v\partial_x u = -\lambda u^p\ ,\ x,t \in [0,L]\times[0,T], \tag{74}$$

where $L = 1$.
The initial condition is defined for $x \in (0,1)$,

$$u(x,0) = \begin{cases} 1\ ,\ x \in (0,1) \\ 0\ ,\ \text{otherwise} \end{cases}. \tag{75}$$

We apply: $u(x,t) = \tilde{u}(\eta)$ and the transformed equation is given as:

$$\begin{cases} -vp\tilde{u}^{-p-1} + vp\ln(\tilde{u}) = -\lambda\eta + C_0(x)\ ,\ \ \eta = x - vt\ ,\ vt \leq x \leq vt+1 \\ 0, \qquad\qquad\qquad\qquad\qquad\qquad else \end{cases}, \tag{76}$$

with $C_0(x)$ is the constant, that can be found with the initial value of $c_0(x)$.
While the initial function is given as:

$$\begin{cases} C_0(x) = -vp\tilde{u}^{-p-1} + vp\ln(\tilde{u}) + \lambda x\ ,\ \ \eta = x\ ,\ 0 \leq x \leq 1 \\ 0, \qquad\qquad\qquad\qquad\qquad\qquad else \end{cases}. \tag{77}$$

Vectorial case

Example 4. We deal with

$$\partial_t u_1^p + v\partial_x u_1 = -\lambda_1 u_1^p \ , \ x, t \in [0, L] \times [0, T], \tag{78}$$
$$\partial_t u_2^p + v\partial_x u_2 = -\lambda_2 u_2^p + \lambda_1 u_1^p \ , \ x, t \in [0, L] \times [0, T], \tag{79}$$

where $L = 10$, $T = 10$.

The initial condition is defined for $x \in (0, 1)$,

$$u_1(x, 0) = \begin{cases} 1 \ , \ x \in (0, 1) \\ 0 \ , \ \text{otherwise} \end{cases} . \tag{80}$$

$$u_2(x, 0) = \begin{cases} 1 \ , \ x \in (0, 1) \\ 0 \ , \ \text{otherwise} \end{cases} . \tag{81}$$

We apply: $u_1(x, t) = \tilde{u}_1(\eta)$, $u_2(x, t) = \tilde{u}_2(\eta)$ and the transformed equation is given as:

$$\begin{cases} -vp\tilde{u}_1^{-p-1} + vp\ln(\tilde{u}_1) & \\ \quad = -\lambda_1 \eta + C_0(x) \ , & \eta = x - vt \ , \ vt \le x \le vt + 1 \ , \\ \qquad 0, & else \end{cases} \tag{82}$$

$$\begin{cases} \qquad -vp\tilde{u}_2^{-p-1} + vp\ln(\tilde{u}_2) & \\ = -\lambda_2 \eta + \lambda_1 \int_0^1 (\frac{\tilde{u}_1}{\tilde{u}_2})^p d\eta + C_1(x) \ , & \eta = x - vt \ , \ vt \le x \le vt + 1 \ , \\ \qquad 0, & else \end{cases} \tag{83}$$

with $C_0(x), C_1(x)$ is the constant, that can be found with the initial value of $u_1(x, 0)$ and $u_2(x, 0)$.

While the initial function is given as:

$$\begin{cases} C_0(x) = -vp\tilde{\tilde{u}}_1^{-p-1} + vp\ln(\tilde{\tilde{u}}_1) + \lambda_1 x \ , & \eta = x \ , \ 0 \le x \le 1 \\ \qquad 0, & else \end{cases} \tag{84}$$

$$\begin{cases} C_1(x) = -vp\tilde{\tilde{u}}_2^{-p-1} + vp\ln(\tilde{\tilde{u}}_2) + \lambda_2 x + \lambda_1 \int_0^1 (\frac{\tilde{u}_1}{\tilde{u}_2})^p dx \ , & \eta = x \ , \ 0 \le x \le 1 \\ \qquad 0, & else \end{cases} \tag{85}$$

where $\tilde{\tilde{u}}_1(\eta) = u_1(x, 0)$, $\tilde{\tilde{u}}_2(\eta) = u_2(x, 0)$. The initial-values can be solved directly.

The full solutions (82) and (83) are solved by a Newton's method.

4 Numerical Experiments

4.1 First experiment: Spatial-dependent Problem

We deal with

$$\partial_t u + (1 + ax)\partial_x u = 0 \ , \ x, t \in [0, L] \times [0, T], \tag{86}$$

where $a = 1$ and $L = 1$, $e(x) = 1 + ax$.
The initial condition is defined for $x \in (0, 1)$,

$$u(x, 0) = \begin{cases} b \ , \ x \in (0, 1) \\ 0 \ , \ \text{otherwise} \end{cases} \ , \tag{87}$$

where $b = 1$,

The transformed equation is given as:

$$\partial_t u + \partial_Z u = 0 \ , \ \ Z, t \in [0, Z_0] \times [0, T], \tag{88}$$

with the initial condition:

$$u(Z, 0) = \begin{cases} b \ , \ Z \in (0, Z_0) \\ 0 \ , \quad \text{otherwise} \end{cases} \ , \tag{89}$$

and $Z = \frac{\ln(1+ax)}{a}$, with $Z_0 = \frac{\ln(1+aL)}{a}$, where $L = 1$.

The solution is given as,

$$u(Z(x), t) = \begin{cases} 0 \ , \quad\quad Z(0) \leq Z(x) \leq Z(t) \\ b \ , \ Z(t) \leq Z(x) \leq Z(t+1) \\ 0 \ , \quad\quad\quad Z(t+1) \leq Z(x) \end{cases} \ , \tag{90}$$

where $b = 1$.

In the following figure 2, we see the spatial-dependent problem.

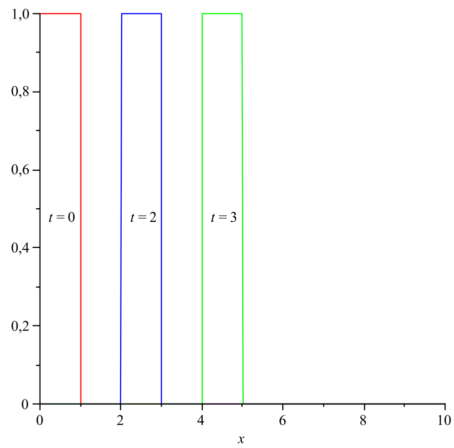

Fig. 2. Experiment with the spatial-dependent problem, here $t = 0.0$.

Remark 2. The results shows the shifted solution of the spatial dependent case. Here we obtain the exact solution with the spatial dependent case.

4.2 Second experiment: descending retardation factor with two species (Transport and Decay)

We use ascending parameters for the retardation factors. The retardation factors are given as $R_1 = 10, R_2 = 0.0$. The reaction factors are given as $\lambda_1 = 2.0, \lambda_2 = 1.8$. Further $g(t) = g_i(t) = t$, $i = 1, \ldots, 2$.

With the assumptions:

- $\lambda_j \neq \lambda_k$
- $v_j \neq v_k$
- $\lambda_{jk} \neq \lambda_{jl}$

The initial conditions are given as

$$\begin{aligned} u_1(x,0) &= \begin{cases} b \ , \ x \in (0,1) \\ 0 \ , \ \text{otherwise} \end{cases} , \\ u_i(x,0) &= 0 \, , \quad i = 2, \ldots, m \ , \end{aligned} \tag{91}$$

where $b = 1$.

The velocity is given as $v = 1$, where each species velocity is given as $v_i = \frac{v}{R_i}$, $i = 1, \ldots, 2$.

The end time is given as $t \in [0, T]$, $T = 10$ and the spacial domain $x \in [0, 10]$.

Here we apply the reduced equation (61) and (62).

The idea is to select the dominated decay chains and to apply them in the scheme.

The spatial-time-dependent cases is given in Figure 3 and 4 .

The mass conserved spatial-timedependent cases of the 2 species is given in the Table 1 and Figure 5

	t=0	t=0.5	t=1	t=2	t=3	t=4	t=6
u_1	1	0.3678794412	0.1353352832	0.007287706133	0	0	0
u_2	0	0.6220667333	0.8428446943	0.8987320224	0.6133217504	0.1865886310	0
$\sum_{i=1}^{2} u_i$	1	0.9899461745	0.9781799775	0.9060197285	0.6133217504	0.1865886310	0

Table 1. Mass conservation of two descending parameters for the spatial-timedependent case.

Remark 3. Here we can see the influence of at least five species to our analytical equations. We can concentrate on the dominant species and save so computational time without loosing accuracy. Such analytical results helps to generalize analytical solutions with efficient computations.

4.3 Nonlinear experiments

In the following experiment, we deal with a nonlinear sorption (Freundlich Isotherm) in equilibrium and apply the equations:

$$\frac{\partial}{\partial t}(\phi u + g(1-\phi)\rho u^p) + q\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = 0 \ \ for x > 0, t > 0 \tag{92}$$

$$u(0,t) = u_0\psi(t), \ \ u(x,0) = 0 \ , \ x > 0, \tag{93}$$

$$with \ \psi(0) = 0 \ and \ \psi(t) \rightarrow 1 \ \ for \ t \rightarrow \infty \tag{94}$$

where $\phi = 0.5$, $q = 0.5$, $D = 0.005$ and $g = 1$.

The exact solution for the equilibrium case are given as:

$$u(x,t) = f(\xi) = u_0(1 - exp(\frac{ab}{a + u_0^{(1-p)}}\frac{(1-p)}{c}\xi))^{\frac{1}{(1-p)}} \quad for \ \xi < 0; \tag{95}$$

$$u(x,t) = f(\xi) = 0.0 \quad for \ \xi \geq 0 \tag{96}$$

$$\xi = x - vt \tag{97}$$

$$v = \frac{bu_0^{(1-p)}}{a + u_0^{(1-p)}} \tag{98}$$

$$a = \frac{g(1-\phi)\rho}{\phi} \quad b = \frac{q}{\phi} \quad c = \frac{D}{\phi} \tag{99}$$

with the inflow-boundary:

$$u(0,t) = u_0\left(1 - exp\left(\frac{ab}{a + u_0^{(1-p)}}\frac{(1-p)}{c}(-\frac{bu_0^{(1-p)}}{a + u_0^{(1-p)}})\right)\right)^{\frac{1}{(1-p)}} \tag{100}$$

The underlying idea is to follow the traveling waves : $\xi = x - vt$, front which is moving in one direction. Such a transformation allows to consider a simpler ODE system and accelerate the solver process.

The numerical are given in Figure 6.

Error between the numerical solution and the exact
solution are given in Figure 7.

Remark 4. A nonlinear experiment is computed with the software UG for different times. Based on fast nonlinear solvers for ordinary differential equations, we could simple extend the idea to a partial differential equation. Such analytical results helps to generalize the nonlinear transport problem to multidimensional applications.

5 Conclusions

We derived analytical solutions of convection dominant equations with spatial and nonlinear dependencies. The spatial-dependent and nonlinear differential equations are transformed to simpler ordinary differential equations, which can be solved analytically.

The analytical test functions can be embedded to discretization methods for the convection diffusion reaction equation.

Further mobile and immobile equations can be treated with decomposition methods that allow to reduce the computational complexity and obtain higher-order discretization schemes.

We could confirm also the new methods with the analytical and numerical test examples and present the higher-order results of the underlying schemes.

In future the decomposition methods and analytically-improved methods can be generalized for non-smooth and non-linear problems in multi-dimensions.

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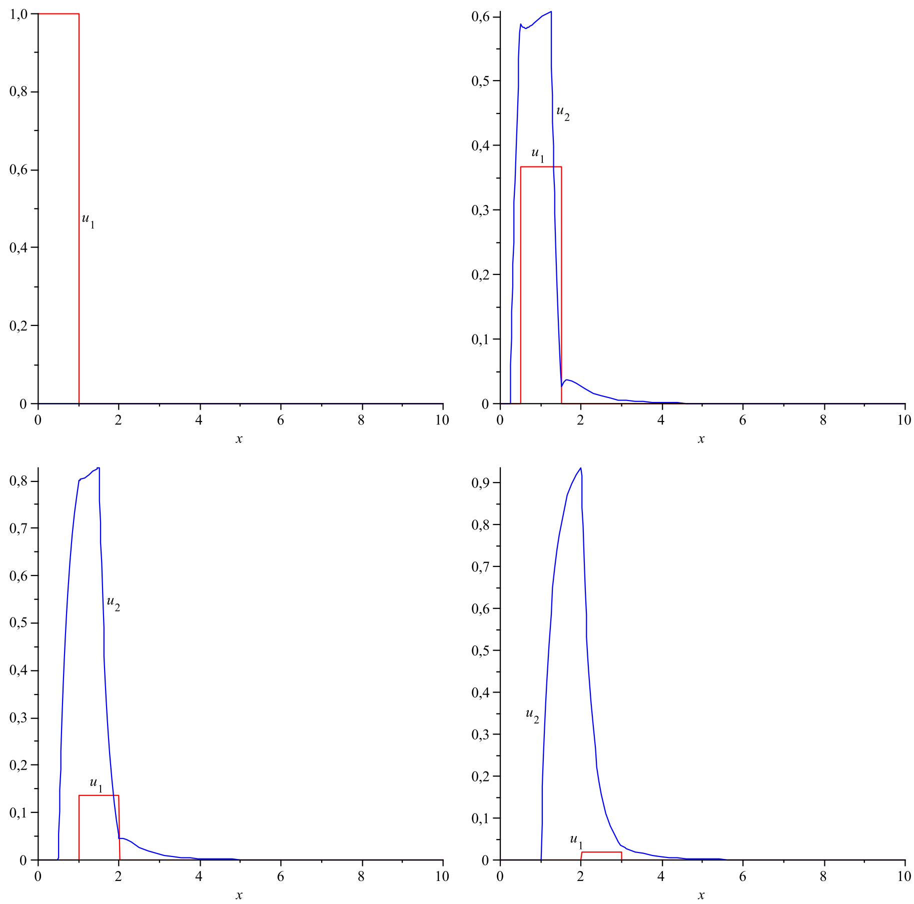

Fig. 3. Experiment with two descending parameters for the spatial-timedependent case with $x \in [0, 1], t \in [0, 3]$.

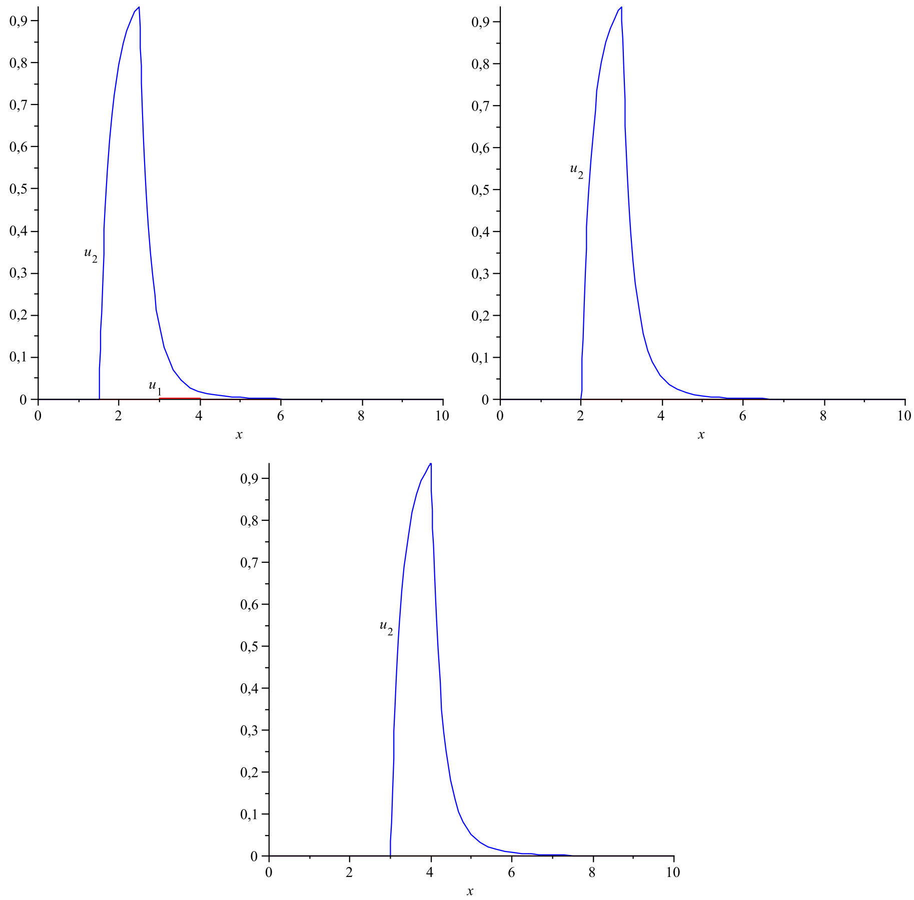

Fig. 4. Experiment with two descending parameters for the spatial-timedependent case with $x \in [0, 1], t \in [3, 6]$.

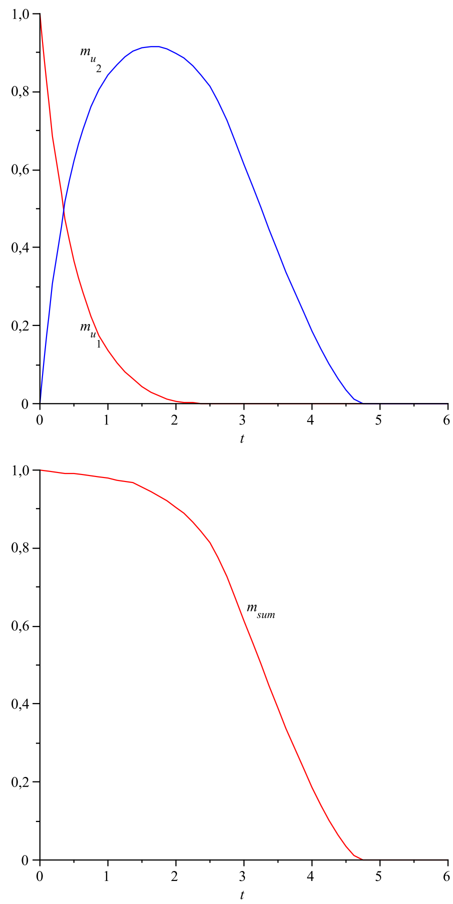

Fig. 5. Experiment with two descending parameters for the spatial-timedependent case in mass conserved version $x \in [0, 1], t \in [0, 6]$.

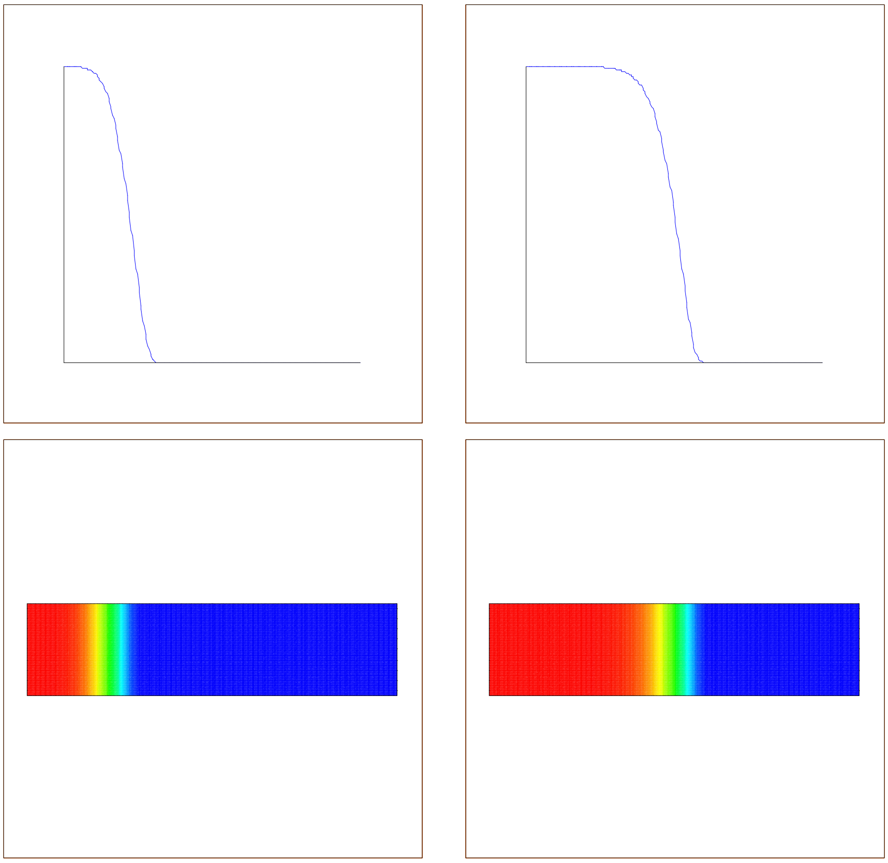

Fig. 6. The traveling of the front Wave after $t = 1$ and $t = 2$.

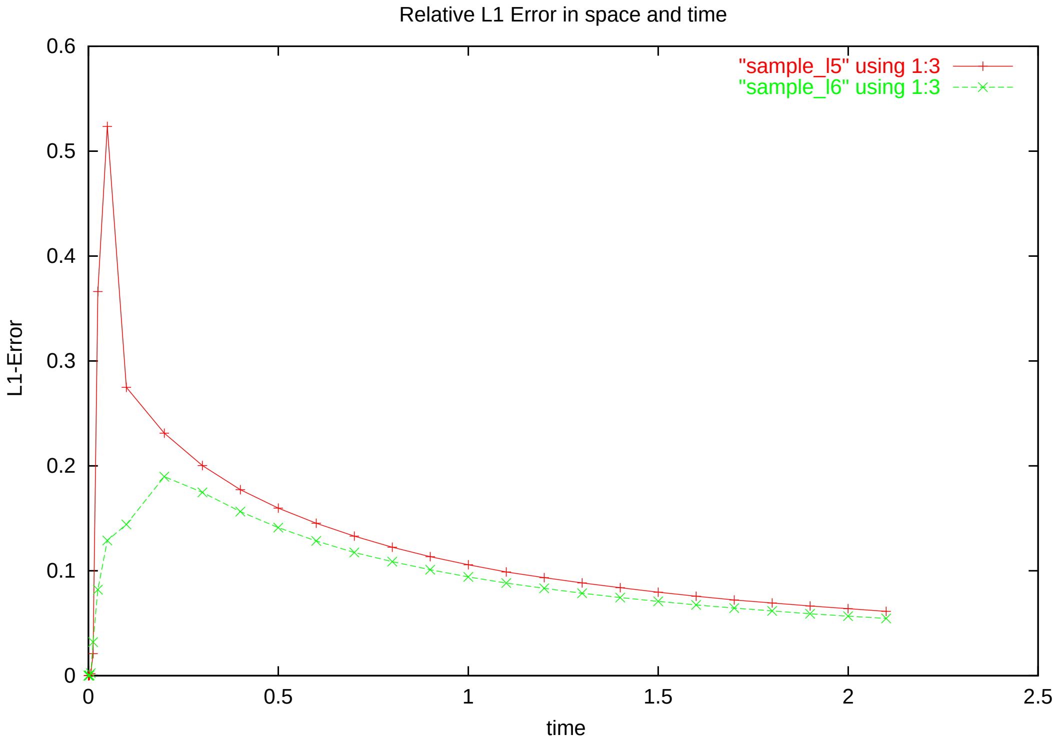

Fig. 7. The relative L1-error for 1 components of the numerical solution of a nonlinear problem in equilibrium.