Discretization methods with analytical solutions for a convection-reaction equation with higher-order discretizations.

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Abstract. We introduce an improved second-order discretization method for the convection-reaction equation by combining analytical and numerical solutions. The method is derived from Godunov's scheme, see [15] and [21], and uses analytical solutions to solve the one-dimensional convection-reaction equation. We can also generalize the second-order methods for discontinuous solutions, because of the analytical test functions. One-dimensional solutions are used in the higher-dimensional solution of the numerical method.
The method is based on the flux-based characteristic methods and is an attractive alternative to the classical higher-order TVD-methods, see [16]. In this article we will focus on the derivation of analytical solutions embedded into a finite volume method, for general and special solutions of the characteristic methods.
For the analytical solution, we use the Laplace transformation to reduce the equation to an ordinary differential equation. With general initial conditions, e.g. spline functions, the Laplace transformation is accomplished with the help of numerical methods. The proposed discretization method skips the classical error between the convection and reaction equation by using the operator-splitting method.
At the end of the article, we illustrate the higher-order method for different benchmark problems. Finally, the method is shown to produce realistic results.

Key words. convection-reaction equation, Godunov's method, Laplace transformation, operator-splitting method, embedded analytical solutions, Finite Volume method, flux-based characteristic method.
AMS subject classifications. 35K15 35K57 47F05 65M60 65N30

1 Introduction

We are motivated to study real-life problems concerning the transport and reaction of radionuclide contaminants in flowing groundwater. Our modeling is based

on homogenization of the underlying porous media, see [3] and [4]. The application of the model to numerical simulations are extensively analyzed and results are presented, for example in [18], [22], and [8]. Because of the delicate problem of simulating large time periods in the real-life simulations, we concentrate on the design of discretization methods to obtain large time steps. We therefore focus on large systems of linearized hyperbolic equations, in our example systems of convection-reaction equations, see [11], [18]. The equations are coupled with the reaction terms and are presented as follows:

$$\partial_t R_i u_i + \nabla \cdot \mathbf{v}\, u_i = -\lambda_i\, R_i\, u_i + \lambda_{i-1}\, R_{i-1}\, u_{i-1} \ \text{ in } \Omega \times (0,T)\,, \tag{1}$$

$$u_{i,0}(x) = u_i(x,0) \ \text{ on } \Omega\,, \tag{2}$$

$$i = 1, \ldots, m\,, \tag{3}$$

where m is the number of equations and i is the index of each component. The unknowns $u_i = u_i(x,t)$ are considered in $\Omega \times (0,T) \subset I\!R^n \times I\!R^+$, where n is the spatial dimension. The retardation factors R_i are constant and $R_i \geq 0$. The reaction part is given with the decay factors λ_i. They are constant and $\lambda_i \geq 0$. For the initialization of the decay chain, we set $\lambda_0 = 0$. The decay chain 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 of the equation is given by the velocity $\mathbf{v} \in I\!R^n$ and is piecewise constant, see [11] and [12].

Here we have a delicate model problem due to the contrasting variation introduced by the very slow flow field and the rapid reaction. Based on this variation, an intensive study of discretization methods is important. The classical methods for pure convection equations are higher-order discretization methods, based on TVD (Total Variation Diminishing) or ENO (Essentially Non-Oscillatory) schemes, see [24] and [25]. Here, the benefit arise from the construction of accurate finite difference and finite volume methods. This is possible due to an approximation that is chosen automatically for the locally smoothest stencil. The reconstruction of these stencils needs flux limiters to obtain the non-oscillatory behavior at the discontinuities, see [25]. Our investigation will focus more on the convection and reaction equations, i.e. the combination of higher-order discretization methods for both the convection and the reaction parts. Towards this end, we contribute a mixed method for the higher-order reconstruction of a finite volume method for the convection portion and analytical solutions of the reaction portion. These concepts were first contributed as Godunov's schemes, see [15], for the pure convection equations. We therefore focus on the analytical solutions of a system of convection-reaction equations and embed these solutions as test functions in our finite volume method, see [9]. The main advantage of such a method is in the treatment of discontinuities, which can be accomplished by piecewise analytical solutions in each finite cell. The keys to the methods for the derivation of analytical solutions, are presented in the paper. For the general case of different parameters and also for the special case of equal pairwise parameters, we introduce analytical solutions. Applications to the spatial discretization,

for example the finite volume scheme, are performed by deriving the analytical solution of the locally mass on a normalized cell. Using the analytical solution of the mass we will detect a new discretization method based on vertex-centered finite volume methods and therefore obtain a multi-dimensional higher-order discretization methods. For the finite volume method, we describe higher-order resolutions that are constructed using Godunov's scheme, see [11]. The higher-order method is limited by the assumptions of the local minimum and maximum principle. For discretization in time, we use an explicit method. The modified method has no time-splitting error and we can confirm the higher convergence order in our numerical results. Based on a triangle impulse we present the improved results. We are not restricted to any shock front in the local cell and a generalization is described in [12]. Another generalization can be accomplished for nonlinear convection-reaction equations, see [18]. We propose a linearization and apply our linear theory of the analytical solutions for one-dimensional convection-reaction equations.

The paper is organized as follows. One of the main contributions is the one-dimensional analytical solution presented in Section 2. The application for general discontinuous solutions with different equation parameters is described in Section 3. In Section 3.3, we construct analytical solutions for the special applications, with pairwise equal parameters presented. The second contribution to the paper is the application of the analytical solutions to the discretization, presented in Section 4. Verification of the new discretization method in various numerical examples is shown in Section 5. We conclude the paper with a discussion of future work.

2 Analytical solutions

In this section, we deal with a system with piecewise constant velocities for coupled transport of contaminants in ground water in one dimension. The equation is given as

$$\partial_t u_i + v_i \partial_x u_i = -\lambda_i u_i + \lambda_{i-1} u_{i-1} \,, \tag{4}$$

for $i = 1, \ldots, m$, whereas m denotes the number of equations. The unknowns $u_i = u_i(x,t)$ denote the contaminant concentrations. They are transported with constant (and in general different) velocities v_i and decay with constant reaction rates λ_i. The spatiotemporal domain is given by $(0,\infty) \times (0,T)$.

We assume a simple (irreversible) form of a decay chain, e.g. $\lambda_0 = 0$, and given single source terms $\lambda_{i-1} u_{i-1}$ for each contaminant. For simplification, we assume that $v_i > 0$ for $i = 1, \ldots, m$. The case $v_i < 0$ can be treated analogously. Due to (4), all velocities v_i must have the same sign and must be piecewise constant for each cell i. Furthermore, we do not allow piecewise equal parameters for the cases $v_i = v_{i-1}$ and $\lambda_i = \lambda_{i-1}$, for $i = 2, \ldots, m$. In the special solutions we will allow these cases.

The analytical solutions for equal retardation factors can be found in [27]. We enlarge the solutions for different retardation factors and for special initial conditions.

We will derive the analytical solutions with piecewise linear initial conditions, although all other piecewise polynomial functions could be derived as shown in the following.

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

$$\begin{aligned} u_1(x,0) &= \begin{cases} ax + b\,, & x \in (0,1) \\ 0 & , \text{otherwise} \end{cases}\,, \\ u_i(x,0) &= 0\,, \quad i = 2, \ldots, m\,, \end{aligned} \tag{5}$$

where a and b are arbitrary constants.

We use the Laplace transformation to translate the partial differential equation to the ordinary differential equation. The transformations for these cases are given in [6], [14] and [17].

In equation (4), we apply the Laplace transformation given in [1] and [5]. For this, we must define the transformed function $\hat{u} = \hat{u}(s,t)$:

$$\hat{u}_i(s,t) := \int_0^\infty u_i(x,t)\, e^{-sx}\, dx\,. \tag{6}$$

Using (4), the functions $\hat{u}_i$ satisfy the transformed equations

$$\partial_t \hat{u}_1 = -\left(\lambda_1 + s v_1\right) \hat{u}_1\,, \tag{7}$$

$$\partial_t \hat{u}_i = -\left(\lambda_i + s v_i\right) \hat{u}_i + \lambda_{i-1} \hat{u}_{i-1}\,, \tag{8}$$

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

$$\hat{u}_1(s,0) = \left(\frac{a}{s^2} + \frac{b}{s}\right)\left(1 - e^{-s}\right) + \frac{a}{s}\, e^{-s}\,, \tag{9}$$

$$\hat{u}_i(s,0) = 0\,, \quad i = 2, \ldots, m\,. \tag{10}$$

We denote for further solutions:

$$\Lambda_i = \prod_{j=1}^{i-1} \lambda_j\,. \tag{11}$$

Equation (8) is solved with the methods for solving ordinary differential equations described in [14]. A more general case is presented in [6].

Thus, we find the exact solution of (7) and (8):

$$\hat{u}_1 = \hat{u}_1(s,0)\, e^{-(\lambda_1 + s v_1)\, t}\,, \tag{12}$$

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

$$\hat{u}_i = \hat{u}_1(s,0)\; \Lambda_i \sum_{j=1}^{i} e^{-(\lambda_j + s v_j) t} \prod_{\substack{k=1 \\ k \neq j}}^{i} \left(s(v_k - v_j) + \lambda_k - \lambda_j\right)^{-1}\,. \tag{13}$$

The analytical solution in (13) can have a singular point for a single value of s, but this causes no difficulties when applying the inverse Laplace transformation.

To obtain the exact solution of (4), we must apply the inverse Laplace transformation to (7), which requires 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

$$\lambda_{kj} = \lambda_{jk} := \frac{\lambda_j - \lambda_k}{v_j - v_k} \,. \tag{14}$$

Furthermore, for the next transformation, we must demand 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

$$\Lambda_{j,i} = \left(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_k - \lambda_j} \right) \,, \quad \Lambda_{jk,i} = \left(\prod_{\substack{l=1 \\ l \neq j \\ l \neq k}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}} \right) \,, \tag{15}$$

where we have the following assumptions:

$$1.\ v_j \neq v_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,, \tag{16}$$
$$2.\ \lambda_j \neq \lambda_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,, \tag{17}$$
$$3.\ \lambda_{jk} \neq \lambda_{jl} \ \ \forall j, k, l = 1, \ldots, m, \text{ for } j \neq k \ \wedge j \neq l \wedge k \neq l, \tag{18}$$
$$4.\ v_j \neq v_k \text{ and } \lambda_j \neq \lambda_k \ \ \forall j, k = 1, \ldots, m, \text{ for } j \neq k \,. \tag{19}$$

Using (15), the last term in (13) for a given index j can be rewritten in the following form,

$$\prod_{\substack{k=1 \\ k \neq j}}^{i} \left(s(v_k - v_j) + \lambda_k - \lambda_j \right)^{-1} = \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{\lambda_{jk}}{s + \lambda_{jk}} \Lambda_{jk,i} \,. \tag{20}$$

Adopting (9) into (12) and (13), the standard inverse Laplace transformation can be used, and the solution u_i for (4) is given by

$$u_1(x,t) = \exp(-\lambda_1 t) \begin{cases} 0 & , 0 \leq x < v_1 t \\ a(x - v_1 t) + b & , v_1 t \leq x < v_1 t + 1 \\ 0 & , v_1 t + 1 \leq x \end{cases} \,, \tag{21}$$

$$u_i(x,t) = \Lambda_i \left(\sum_{j=1}^{i} \exp(-\lambda_j t) \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \Lambda_{jk,i} A_{jk} \right) \,, \tag{22}$$

$$A_{jk} = \begin{cases} 0 & , 0 \le x < v_j t \\ a(x - v_j t) & \\ +(b - \frac{a}{\lambda_{jk}})(1 - \exp(-\lambda_{jk}(x - v_j t))) & , v_j t \le x < v_j t + 1 \\ (b - \frac{a}{\lambda_{jk}} + a)\exp(-\lambda_{jk}(x - v_j t - 1)) & \\ -(b - \frac{a}{\lambda_{jk}})\exp(-\lambda_{jk}(x - v_j t)) & , v_j t + 1 \le x \end{cases} . \quad (23)$$

Because of the numerical computation required for the analytical solution, we have derived an improved notation for equations (21) and (22) to avoid numerical instabilities.

The improved solutions, cf. [11], with the new notation are given as

$$u_i(x,t) = \Lambda_i \sum_{j=1}^{i} \left(L_{j,i} + \sum_{k>j}^{i} \begin{cases} M_{jk,i} & , v_j < v_k \\ M_{kj,i} & , v_k < v_j \\ 0 & , \text{otherwise} \end{cases} \right) , \quad (24)$$
$$\text{with} \quad i = 2, \ldots, m ,$$

where the factors $L_{j,i}$ and $M_{jk,i}$ are defined as:

$$L_{j,i} := \begin{cases} \exp(-\lambda_j t)\ \Lambda_{j,i} \left(a(x - v_j t) + b \right. & \\ \left. -a \sum_{\substack{k=1 \\ k \ne j}}^{i} \frac{1}{\lambda_{jk}} \right) & , v_j t \le x \le v_j t + 1 \\ 0 & , \text{otherwise} \end{cases} , \quad (25)$$

$$M_{jk,i} := \begin{cases} \Lambda_{j,i}\ \Lambda_{jk,i}\ g_{jk} & , v_j t \le x \le v_k t \\ \Lambda_{j,i}\ \Lambda_{jk,i}\ h_{jk} & , v_j t + 1 \le x \le v_k t + 1 \\ 0 & , \text{otherwise} \end{cases} , \quad (26)$$

and the factors g_{jk} and h_{jk} are given as

$$g_{jk} := -(b - \frac{a}{\lambda_{jk}})\exp(-\lambda_j t)\exp(-\lambda_{jk}(x - v_j t)) , \quad (27)$$

$$h_{jk} := (b - \frac{a}{\lambda_{jk}} + a)\exp(-\lambda_j t)\exp(-\lambda_{jk}(x - v_j t - 1)) . \quad (28)$$

In the next section, we apply solution (24) to the first and second component.

3 General solution

3.1 The first component

The first component u_1 of the solution for (4) is trivial and well-known; we repeat it here to give a complete presentation:

$$u_1(x,t) = \begin{cases} (a(x - v_1 t) + b)\ e^{-\lambda_1 t} & , v_1 t \le x \le v_1 t + 1 \\ 0 & , \text{otherwise} \end{cases} . \quad (29)$$

3.2 The second component

For the second component, we use the equation (24) with the improved notation and obtain the result as follows.

The second component u_2 of the solution for (4) is given as

$$u_2(x,t) = \lambda_1 \left(L_{1,2} + L_{2,2} + \begin{cases} M_{12,2} \text{ , } v_1 < v_2 \\ M_{21,2} \text{ , } v_2 < v_1 \\ 0 \quad \text{ , sonst} \end{cases} \right), \tag{30}$$

where $\lambda_1 \neq \lambda_2$ and $v_1 \neq v_2$ are given.

The factors of equation (30) are given by

$$L_{1,2} = \begin{cases} \exp(-\lambda_1 t)\frac{1}{\lambda_2-\lambda_1}(a(x-v_1t)+b-a\frac{1}{\lambda_{12}}) \text{ , } v_1t \leq x \leq v_1t+1 \\ 0 \quad \text{ , otherwise} \end{cases},$$

$$L_{2,2} = \begin{cases} \exp(-\lambda_2 t)\frac{1}{\lambda_1-\lambda_2}(a(x-v_2t)+b-a\frac{1}{\lambda_{12}}) \text{ , } v_2t \leq x \leq v_2t+1 \\ 0 \quad \text{ , otherwise} \end{cases},$$

$$M_{12,2} = \begin{cases} \exp(-\lambda_1 t)\frac{1}{\lambda_2-\lambda_1}(-b+a\frac{1}{\lambda_{12}}) \\ \cdot \exp(-\lambda_{12}(x-v_1t)) \quad \text{ , } v_1t \leq x \leq v_2t \\ \exp(-\lambda_1 t)\frac{1}{\lambda_2-\lambda_1}(b-a\frac{1}{\lambda_{12}}+a) \\ \cdot \exp(-\lambda_{12}(x-v_1t-1)) \quad \text{ , } v_1t+1 \leq x \leq v_2t+1 \\ 0 \quad \text{ , otherwise} \end{cases},$$

$$M_{21,2} = \begin{cases} \exp(-\lambda_2 t)\frac{1}{\lambda_1-\lambda_2}(-b+a\frac{1}{\lambda_{12}}) \\ \cdot \exp(-\lambda_{12}(x-v_2t)) \quad \text{ , } v_2t \leq x \leq v_1t \\ \exp(-\lambda_2 t)\frac{1}{\lambda_1-\lambda_2}(b-a\frac{1}{\lambda_{12}}+a) \\ \cdot \exp(-\lambda_{12}(x-v_2t-1)) \quad \text{ , } v_2t+1 \leq x \leq v_1t+1 \\ 0 \quad \text{ , otherwise} \end{cases}.$$

For more than two components, we could use equation (24) and compute the factors numerically. The additive behavior of the equations can be used for the efficient numerical computation of the solutions.

3.3 Special solutions

We now introduce the special solutions and focus on equal, pairwise parameters. For a more general case, we can derive the special solutions as presented below.

For the analytical solution, we focus on the case $\lambda_l = \lambda_{a(l)}$ with $l \neq a(l)$.

Special solution for the case $\boldsymbol{\lambda_l = \lambda_{a(l)}}$ For the equal, pairwise parameters $\lambda_l = \lambda_{a(l)}$, we derive the solution with the transformed equation (13) and eliminate the zero terms $\lambda_l - \lambda_{a(l)}$, see also the derivations in [17].

We get the following equations for the special case in which $\lambda_l = \lambda_{a(l)}$.

$$\begin{aligned}\hat{u}_i(s,t) = \hat{u}_1(s,0)\ \Lambda_i \qquad (31)\\ \cdot \Bigg(\exp(-(\lambda_l + s v_l)t) \frac{1}{s(v_{a(l)} - v_l)} \prod_{\substack{k=1\\k\neq l\\k\neq a(l)}}^{i} \frac{1}{s(v_k - v_l) + (\lambda_k - \lambda_l)}\\ + \exp(-(\lambda_{a(l)} + s v_{a(l)})t) \frac{1}{s(v_l - v_{a(l)})} \prod_{\substack{k=1\\k\neq a(l)\\k\neq l}}^{i} \frac{1}{s(v_k - v_{a(l)}) + (\lambda_k - \lambda_{a(l)})}\\ + \sum_{\substack{j=1\\j\neq l\\j\neq a(l)}}^{i} \exp(-(\lambda_j + s v_j)t) \prod_{\substack{k=1\\k\neq j}}^{i} \frac{1}{s(v_k - v_j) + (\lambda_k - \lambda_j)} \Bigg).\end{aligned}$$

For the retransformation into the original space of the solution, we rearrange equation (31) with the help of equation (20). We rewrite equation (31) and get the following different cases.

Case 1: $i = 2$ and $(l, a(l)) = (1, 2)$

$$\begin{aligned}\hat{u}_2 = \hat{u}_1(s,0)\ \lambda_1 \qquad (32)\\ \cdot \Big(\exp(-(\lambda_1 + v_1 s)t)\ \frac{1}{v_2 - v_1}\ \frac{1}{s} + \exp(-(\lambda_2 + v_2 s)t)\ \frac{1}{v_1 - v_2}\ \frac{1}{s} \Big).\end{aligned}$$

Case 2: $i = 3, \ldots, m$

$$\begin{aligned}\hat{u}_i = \hat{u}_1(s,0)\ \Lambda_i \qquad (33)\\ \cdot \Bigg(\exp(-(\lambda_l + v_l s)t)\ \frac{1}{v_{a(l)} - v_l}\ \Lambda_{l,a(l),i}\ \frac{1}{s} \sum_{\substack{k=1\\k\neq l\\k\neq a(l)}}^{i} \Lambda_{lk,a(l),i}\ \frac{\lambda_{lk}}{s + \lambda_{lk}}\\ + \exp(-(\lambda_{a(l)} + v_{a(l)} s)t)\ \frac{1}{v_l - v_{a(l)}}\ \Lambda_{a(l),l,i}\ \frac{1}{s} \sum_{\substack{k=1\\k\neq a(l)\\k\neq l}}^{i} \Lambda_{a(l)k,l,i}\ \frac{\lambda_{a(l)k}}{s + \lambda_{a(l)k}}\\ + \sum_{\substack{j=1\\j\neq l\\j\neq a(l)}}^{i} \exp(-(\lambda_j + v_j s)t)\ \Lambda_{j,i} \sum_{\substack{k=1\\k\neq j}}^{i} \Lambda_{jk,i}\ \frac{\lambda_{jk}}{s + \lambda_{jk}} \Bigg),\end{aligned}$$

where the factors Λ_i, $\Lambda_{j,i}$ and $\Lambda_{jk,i}$ are defined in equations (11) and (15). The new factors $\Lambda_{l,a(l),i}$, $\Lambda_{a(l),l,i}$, $\Lambda_{lk,a(l),i}$ and $\Lambda_{a(l)k,l,i}$ are denoted as

$$\Lambda_{l,a(l),i} = \prod_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \frac{1}{\lambda_k - \lambda_l}\ ,\ \Lambda_{a(l),l,i} = \prod_{\substack{k=1 \\ k\neq a(l) \\ k\neq l}}^{i} \frac{1}{\lambda_k - \lambda_{a(l)}}\ , \tag{34}$$

$$\Lambda_{lk,a(l),i} = \prod_{\substack{n=1 \\ n\neq k \\ n\neq l \\ n\neq a(l)}}^{i} \frac{\lambda_{ln}}{\lambda_{ln} - \lambda_{lk}}\ ,\ \Lambda_{a(l)k,l,i} = \prod_{\substack{n=1 \\ n\neq k \\ n\neq a(l) \\ n\neq l}}^{i} \frac{\lambda_{a(l)n}}{\lambda_{a(l)n} - \lambda_{a(l)k}}\ . \tag{35}$$

The retransformation is accomplished with the help of retransformable analytical solutions, cf. [19].
For equation (33), we get the following results.
Case 2: $i = 3, \ldots, m$

$$\begin{aligned} u_i = {} & \Lambda_i \\ & \cdot \Bigg(\frac{1}{v_{a(l)} - v_l} \exp(-\lambda_l t)\ \Lambda_{l,a(l),i} \sum_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \Lambda_{lk,a(l),i}\ (\alpha_l - \frac{A_{lk}}{\lambda_{lk}}) \\ & + \frac{1}{v_l - v_{a(l)}} \exp(-\lambda_{a(l)} t)\ \Lambda_{a(l),l,i} \sum_{\substack{k=1 \\ k\neq a(l) \\ k\neq l}}^{i} \Lambda_{a(l)k,l,i}\ (\alpha_{a(l)} - \frac{A_{a(l)k}}{\lambda_{a(l)k}}) \\ & + \sum_{\substack{j=1 \\ j\neq l \\ j\neq a(l)}}^{i} \exp(-\lambda_j t)\ \Lambda_{j,i} \sum_{\substack{k=1 \\ k\neq j}}^{i} \Lambda_{jk,i}\ A_{jk} \Bigg). \end{aligned} \tag{36}$$

where the terms A_{jk} are given in equation (23). The factor α_l is defined as

$$\alpha_l = \begin{cases} 0 & 0 \le x < v_l t \\ a\frac{(x - v_l t)^2}{2} + b(x - v_l t) & v_l t \le x < v_l t + 1 \\ a\frac{1}{2} + b & v_l t + 1 \le x \end{cases}. \tag{37}$$

We analogously define $\alpha_{a(l)}$ by changing l by $a(l)$.

A further simplification is made possible by rearranging the factor α_l in equation (36), and we get the following equations for the two cases.

Case 1: $i = 2$ and $(l, a(l)) = (1, 2)$

$$u_2 = \lambda_1 \exp(-\lambda_1 t) \left(\frac{1}{v_2 - v_1}\ \alpha_1 + \frac{1}{v_1 - v_2}\ \alpha_2 \right). \tag{38}$$

Case 2: $i = 3, \ldots, m$

$$u_i = \Lambda_i \tag{39}$$

$$\cdot \left(\frac{1}{v_{a(l)} - v_l} \exp(-\lambda_l t)\, \Lambda_{l,a(l),i} \left(\alpha_l - \sum_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \Lambda_{lk,a(l),i}\, \frac{A_{lk}}{\lambda_{lk}} \right) \right.$$

$$+ \frac{1}{v_l - v_{a(l)}} \exp(-\lambda_{a(l)} t)\, \Lambda_{a(l),l,i} \left(\alpha_{a(l)} - \sum_{\substack{k=1 \\ k\neq a(l) \\ k\neq l}}^{i} \Lambda_{a(l)k,l,i}\, \frac{A_{a(l)k}}{\lambda_{a(l)k}} \right)$$

$$\left. + \sum_{\substack{j=1 \\ j\neq l \\ j\neq a(l)}}^{i} \exp(-\lambda_j t)\, \Lambda_{j,i} \sum_{\substack{k=1 \\ k\neq j}}^{i} \Lambda_{jk,i}\, A_{jk} \right),$$

where equation (40) (below) is used for the rearrangement

$$\sum_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \Lambda_{lk,a(l),i} = 1\,. \tag{40}$$

This can be performed with complete induction; for comparison see [11].

For the numerical computation, we reformulate solution (39) with a notation that skips numerical instabilities for the interval boundaries $\max_{l=1,\ldots,i}\{v_l+1\} \leq x$.

The reformulations of solutions (38) and (39) are given below for both cases.

Case 1: $i = 2$ and $(l, a(l)) = (1, 2)$

$$u_2(x,t) = \lambda_1 \begin{cases} N_{1,2,2} & v_1 < v_2 \\ N_{2,1,2} & v_2 < v_1 \\ 0 & sonst \end{cases}. \tag{41}$$

Case 2: $i = 3, \ldots, m$

$$u_i(x,t) = \prod_{j=1}^{i-1} \lambda_j \left(\sum_{\substack{j=1 \\ j\neq l \\ j\neq a(l)}}^{i} L_{j,i} + \sum_{j=1}^{i} \sum_{\substack{k>j \\ (j,k)\neq(l,a(l))}}^{i} \begin{cases} M_{jk,i} & v_j < v_k \\ M_{kj,i} & v_k < v_j \\ 0 & sonst \end{cases} \right. \tag{42}$$

$$\left. + P_{l,i} + P_{a(l),i} + \begin{cases} N_{l,a(l),i} & v_l < v_{a(l)} \\ N_{a(l),l,i} & v_{a(l)} < v_l \\ 0 & \text{otherwise} \end{cases} \right),$$

where the factors $L_{j,i}$, $M_{jk,i}$ and $M_{kj,i}$ are given in equations (25) and (26).

The factors $P_{l,i}$, $P_{a(l),i}$, $N_{l,a(l),i}$ and $N_{a(l),l,i}$ are denoted as follows:

$$P_{l,i} = -\exp(-\lambda_l t)\, \frac{1}{v_{a(l)} - v_l}\, \Lambda_{l,i} \begin{cases} c_{l,i} & v_l t \leq x \leq v_l t + 1 \\ 0 & sonst \end{cases}, \tag{43}$$

where the factor $c_{l,i}$ is given as:

$$c_{l,i} = (a(x - v_l t) + b) \sum_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \frac{1}{\lambda_{lk}} - a \sum_{\substack{k=1 \\ k\neq l \\ k\neq a(l)}}^{i} \left(\frac{1}{\lambda_{lk}} \sum_{\substack{n\geq k \\ n\neq l \\ n\neq a(l)}}^{i} \frac{1}{\lambda_{ln}} \right). \tag{44}$$

The factor $c_{a(l)}$ is given analogously.

The factor $N_{l,a(l),i}$ is given by the following equation:

$$N_{l,a(l),i} = \frac{1}{v_{a(l)} - v_l} \exp(-\lambda_l t)\ \Lambda_{l,i} \left(\begin{cases} d_l & v_l t \le x \le v_l t + 1 \\ e & v_l t + 1 \le x \le v_{a(l)} t + 1 \\ 0 & sonst \end{cases} - \begin{cases} d_{a(l)} & v_{a(l)} t \le x \le v_{a(l)} t + 1 \\ 0 & sonst \end{cases} \right), \tag{45}$$

where the equality of $\Lambda_{l,i} = \Lambda_{a(l),i}$ is used.

The factors d_l, e are denoted by:

$$d_l = a\ \frac{(x - v_l t)^2}{2} + b\ (x - v_l t)\ , \tag{46}$$

$$e = a\ \frac{1}{2} + b\ , \tag{47}$$

where the factor $d_{a(l)}$ can be derived by resetting l with $a(l)$.

The derivation of the new notation is performed in [11]. For multiple reactions in the irreversible case, we can enlarge the cases using the methods found in [6].

3.4 Mass reconstruction

In this section, the solution of the mass is described. We present the integration over different intervals and obtain the analytical mass with further simplifications. For the analytical solution of the mass, which is used in the new discretization method, we use the following assumption. The mass is derived in the norm interval $(0, 1)$ and the total mass is given by

$$m_{i,sum}(t) = m_{i,rest}(t) + m_{i,out}(t)\ . \tag{48}$$

We derive the mass $m_{i,rest}(t)$, which is found in the interval $(0, 1)$. Because of the piecewise independent solution, given with $u_i = \sum_{j=1}^{i} u_{ij}$, we can compute $m_{i,rest}(t)$ piecewise in the underlying intervals:

$$\begin{aligned} m_{i,rest}(t) &= \int_{\min_{j=1}^{i}(v_j t)}^{1} u_i(x,t)dx \\ &= \sum_{j=1}^{i} \int_{v_j t}^{1} u_{ij}(x,t)dx\ . \end{aligned} \tag{49}$$

The mass is integrated over the subintervals:

$$m_{i,rest}(t) = \frac{R_1}{R_i}\ \Lambda_i \left(\sum_{j=1}^{i} \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} \Lambda_{jk,i} \exp(-\lambda_j t) \right) \tag{50}$$

$$\cdot \int_{v_j t}^{1} \left(a(x - v_j t) + (b - \frac{a}{\lambda_{jk}})(1 - \exp(-\lambda_{jk}(x - v_j t))) \right) dx \ ,$$
$$\text{with} \quad i = 2, \ldots, m \ ,$$

where the factors Λ_i , $\Lambda_{j,i}$ and $\Lambda_{jk,i}$ are given in (11) and (15).

We could derive a simpler and more compressed form of equation 50 with the following assumptions:

a) The polynomials with constant factors can be reduced to:

$$\sum_{\substack{k=1 \\ k \neq j}}^{i} (\prod_{\substack{l=1 \\ l \neq k \\ l \neq j}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}}) 1 = 1 \ . \tag{51}$$

b) The polynomials with linear factors can be reduced to:

$$\sum_{\substack{k=1 \\ k \neq j}}^{i} (\prod_{\substack{l=1 \\ l \neq k \\ l \neq j}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}}) \frac{1}{\lambda_{jk}} = \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}} \ . \tag{52}$$

c) The polynomials with quadratic factors can be reduced to:

$$\sum_{\substack{k=1 \\ k \neq j}}^{i} (\prod_{\substack{l=1 \\ l \neq k \\ l \neq j}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}}) \frac{1}{(\lambda_{jk})^2} = \sum_{\substack{k=1 \\ k \neq j}}^{i} (\frac{1}{\lambda_{jk}} \sum_{\substack{l \geq k \\ l \neq j}}^{i} \frac{1}{\lambda_{jl}}) \ . \tag{53}$$

d) The symmetry of the exponential terms is given by:

$$\exp(-\lambda_j t) \exp(\lambda_{jk}(1 - v_j t)) = \exp(-\lambda_k t) \exp(-\lambda_{kj}(1 - v_k t)) \ . \tag{54}$$

By using assumptions (51) - (54), we can reduce equation (50) to obtain an applicable form:

$$\begin{aligned} m_{i,rest}(t) = \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} & \\ \cdot \exp(-\lambda_j t) & \left(a \frac{(1 - v_j t)^2}{2} + b(1 - v_j t - \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) \right. \\ & \left. - a(1 - v_j t)(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) + a \left(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}} (\sum_{\substack{l \geq k \\ l \neq j}}^{i} \frac{1}{\lambda_{jl}}) \right) \right) \ , \end{aligned} \tag{55}$$

where the factors Λ_i and $\Lambda_{j,i}$ are given in (11) and (15).

The out-flowing mass $m_{i,out}(t)$, that leaves the norm interval $(0, 1)$, is denoted

$$m_{i,out}(t) = m_{i,sum}(t) - m_{i,rest}(t) \ . \tag{56}$$

Thus, we derive the total mass, which is the mass of the initial impulse $u_i(x,0)$ multiplied by the decay of component i.

The proof is given as follows:
We order the velocities with the notation of the permutation $v_{k(1)} < \ldots < v_{k(i)}$, and, without a restriction, we use the order $v_1 < v_2 < \ldots < v_i$. We can then compute the mass

$$\begin{aligned} m_{i,sum}(t) &= \int_{\min_{j=1}^{i}(v_j t)}^{1+\max_{j=1}^{i}(v_j t)} u_i(x,t)dx \\ &= \sum_{j=1}^{i} \int_{v_j t}^{1+v_j t} u_{ij}(x,t)dx + \sum_{j=1}^{i-1} \int_{1+v_j t}^{1+v_i t} u_{ij}(x,t)dx. \end{aligned} \tag{57}$$

The integration satisfies the equation

$$\begin{aligned} m_{i,sum}(t) = \frac{R_1}{R_i}\, \Lambda_i \Bigg(& \sum_{j=1}^{i}\, \Lambda_{j,i} \sum_{\substack{k=1 \\ k\neq j}}^{i}\, \Lambda_{jk,i} \exp(-\lambda_j t) \\ & \cdot\Bigg(a\, \frac{1}{2} + (b - \frac{a}{\lambda_{jk}})(1 + \frac{1}{\lambda_{jk}}\, (\, \exp(-\lambda_{jk}1) - 1)\,)\Bigg)\Bigg) \\ + \frac{R_1}{R_i}\, \Lambda_i \Bigg(& \sum_{j=1}^{i-1} \Lambda_{j,i} \sum_{\substack{k=1 \\ k\neq j}}^{i} \Lambda_{jk,i}\ \exp(-\lambda_j t) \\ & \cdot\Bigg((b - \frac{a}{\lambda_{jk}} + a)(-\frac{1}{\lambda_{jk}}(\exp(-\lambda_{jk}(v_i - v_j)t) - 1)) \\ & -(b - \frac{a}{\lambda_{jk}})(-\frac{1}{\lambda_{jk}}(\exp(-\lambda_{jk}((v_i - v_j)t + 1)) - \exp(-\lambda_{jk}1)))\Bigg)\Bigg), \end{aligned} \tag{58}$$

where the factors Λ_i, $\Lambda_{j,i}$ and $\Lambda_{jk,i}$ are given in (11) and (15).

We use assumptions (51) - (54) and can reduce equation (58) into a simpler form:

$$m_{i,sum}(t) = f_i^n\ (a\frac{1}{2} + b)\ , \tag{59}$$

$$f_i^n(t) = \frac{R_1}{R_i}\, \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i}\ \exp(-\lambda_j t)\ . \tag{60}$$

For further calculations we define the following masses with parameters:

$$m_{i,out}(\tau^n) = m_{i,out}(a, b, \tau^n, v_1, \ldots, v_i, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i)\ , \tag{61}$$

$$m_{i,sum}(\tau^n) = m_{i,sum}(a, b, \tau^n, v_1, \ldots, v_i, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i)\ , \tag{62}$$

$$f_i^n(\tau^n) = f(\tau^n, v_1, \ldots, v_i, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i)\ . \tag{63}$$

4 Discretization

For the standard method, we use a finite volume method with a higher-order reconstruction for the convection equation. For the reaction term in the standard method, we use the analytical solution for the ordinary differential equation. The results are coupled with the operator-splitting method. In the modified method, we use the discretization of the convection equation and embed the analytical solution of the one-dimensional convection-reaction equation to skip the splitting error.

We introduce all of these methods in this section.

4.1 Notation for discretization methods

The notation of the finite volume method is given below:

For the time steps we use the interval $(t^n, t^{n+1}) \subset (0, T)$, for $n = 0, 1, \ldots, N$. N is the number of time intervals. The computational cells are denoted with $\Omega_j \subset \Omega$, for $j = 1, \ldots, I$. I is the number of nodes on the dual mesh and is unknown.

To use the finite volumes, we construct the dual mesh for the triangulation $\mathcal{T}$ of the domain Ω, cf. [11]. The finite elements for the domain Ω are $T^e, e = 1, \ldots, E$, where E denotes the number of elements. The polygonal computational cells Ω_j are related to the vertices x_j of the triangulation.

The volume of each cell and the relation between neighboring cells is introduced in the following notation.
$V_j = |\Omega_j|$ is the volume of cell j. The set Λ_k denotes the neighboring points x_k of the point x_j. The boundary segments Γ_{jk}, with $j \neq k$, are given with $\Omega_j \cap \Omega_k$.

We define the flux over the boundary Γ_{jk} as

$$v_{jk} = \int_{\Gamma_{jk}} \mathbf{n} \cdot \mathbf{v} \, ds \, . \tag{64}$$

The inflow flux is given as $v_{jk} < 0$ and the outflow flux is $v_{jk} > 0$. The antisymmetric behavior of the fluxes is given by $v_{jk} = -v_{kj}$. The total outflow flux is given by

$$\nu_j = \sum_{k \in out(j)} v_{jk}. \tag{65}$$

The finite volume discretization constructs an algebraic system of equations to express the unknown $u_j^n \approx u(x_j, t^n)$. The initial values are given with u_i^0. The expression of the interpolation schemes may be given naturally in two ways. The first is given with the primary mesh of the finite elements,

$$u^n = \sum_{j=1}^{I} u_j^n \phi_j(x) \, , \tag{66}$$

with ϕ_j being the standard globally finite element basis functions [9]. The second possibility for the finite volumes is given by

$$\hat{u}^n = \sum_{j=1}^{I} u_j^n \varphi_j(x) \ , \tag{67}$$

where φ_j are constant, piecewise, and discontinuous functions defined by $\varphi_j(x) = 1$ for $x \in \Omega_j$ and $\varphi_j(x) = 0$ otherwise.

4.2 First-order finite volume discretization

We introduce the finite volume discretization for the convection equation. The equation is given by

$$\partial_t R u - \mathbf{v} \cdot \nabla u = 0 \ \text{ in } \Omega \times [0,T] \ , \tag{68}$$

$$u_0(x) = u(x,0) \ \text{ on } \Omega \ , \tag{69}$$

where R is constant and $\mathbf{v}$ is the piecewise constant velocity. We use the simple boundary condition $u = 0$ for the inflow and outflow boundary. We use the upwind discretization done in [9] and get

$$R\, V_j \ u_j^{n+1} = u_j^n (R\, V_j - \tau^n \nu_j) + \tau^n \sum_{l \in in(j)} R\, u_l^n \ v_{lj} \ . \tag{70}$$

To satisfy the discrete minimum-maximum property, cf. [9], we have to restrict the time step, if we have the following case:

$$\tau_j^n = \frac{R\, V_j}{\nu_j} \ , \tag{71}$$

$$\tau^n \leq \min_{j=1,\ldots,I} \tau_j^n \ . \tag{72}$$

The second-order discretization is introduced in the following subsection with a reconstruction by linear polynomials.

4.3 Second-order finite volume discretization

Now we reconstruct a second-order discretization scheme, where the linear interpolation scheme is used for the numerical solutions.

The reconstruction is performed in paper [9]. We explain the method in the following steps. We use the following definitions for the element-wise gradient to define the linear construction:

$$c^n(x_j) = u_j^n \ , \tag{73}$$

$$\nabla c^n|_{V_j} = \frac{1}{V_j} \sum_{e=1}^{E} \int_{T^e \cap \Omega_j} \nabla u^n dx \ , \tag{74}$$

$$\text{with} \quad j = 1, \ldots, I \ .$$

The piecewise linear function is given by

$$c_{jk}^n = u_j^n + \psi_j \nabla c^n|_{V_j}(x_{jk} - x_j) \,, \quad \text{with} \quad j = 1, \ldots, I \,, \tag{75}$$

where $\psi_j \in (0,1)$ is the limiter, which must satisfy the discrete minimum-maximum property. For the outflow boundary of the finite cell, with c_{jk}^n, $k \in out(j)$, the next condition that must satisfied is:

$$\min\{u_j^n, u_l^n, l \in in(j)\} \leq c_{jk}^n \leq \max\{u_j^n, u_l^n, l \in in(j)\} \,. \tag{76}$$

For the inflow boundary of the finite cell, with $c_{jk'}^n$, $k' \in in(j)$, the following condition must be satisfied:

$$\min\{u_j^n, u_l^n, l \in in(j)\} \leq c_{jk'}^n \leq \max\{u_j^n, u_l^n, l \in in(j)\} \,. \tag{77}$$

The time step is restricted with the following expression

$$\frac{\tau^n}{R\, V_j} \leq \nu_j^{-1} \min_{k \in out(j)} \alpha_{jk}^n \,, \tag{78}$$

where the parameter α_{jk}^n is defined as

$$\alpha_{jk}^n = \frac{u_j^n - c_{jk'}^n}{c_{jk}^n - c_{jk'}^n} \,. \tag{79}$$

To enable a maximal time step τ^n for the method, we replace c_{jk}^n by the time-step-dependent value,

$$c_{jk}^n(\tau^n) := c_{jk}^n + \frac{\tau^n}{\tau_j} \left(u_j^n - c_{jk}^n\right) . \tag{80}$$

The proof for the local min-max property is given in [9].

Using all the previous schemes, the second-order discretization can be written in the form

$$R\, V_j\; u_j^{n+1} = R\, V_j\; u_j^n - \tau^n \sum_{k \in out(j)} c_{jk}^n(\tau^n)\; v_{jk} + \tau^n \sum_{l \in in(j)} c_{lj}^n(\tau^n)\; v_{lj}. \tag{81}$$

4.4 Operator-splitting method and standard discretization

In this subsection, the higher-order discretization we derived for the convection equation is used for the standard and modified method.

The operator-splitting methods we used are based on the first-order methods, cf. [29]. For the operator A we use the reaction equation and solve it exactly (we have already shown this in [10]). For the operator B we use the discretization of the convection term as described in the previous sections.

The standard discretization uses the following operator-splitting method,

$$\partial_t c = A\ c + B\ c\ ,$$

where the initial conditions are $c(t^n) = c^n$. The first-order splitting method is accomplished with

$$\begin{aligned}
&\partial_t c^* = Ac^* \quad \text{with} \quad c^*(t^n) = c^n\ , \\
&\partial_t c^{**} = Bc^{**} \quad \text{with} \quad c^{**}(t^n) = c^*(t^{n+1})\ ,
\end{aligned}$$

where the result of the methods are $c(t^{n+1}) = c^{**}(t^{n+1})$. The operators A and B do not commute because of their different retardation factors, cf. [29]. Therefore we have a splitting error of first-order $O(\tau^n)$. We could improve our results with a second-order splitting method, the so-called *Strang splitting method*, described in [26], where the error is $O((\tau^n)^2)$.

4.5 Modified discretization with finite volume methods of higher-order and embedded analytical solutions

We now apply a Godunov's method for the discretization. We reduce the equation to a one-dimensional problem, solve the equation exactly, and transform the one-dimensional mass to the multi-dimensional equation. Therefore, we only get an error in the spatial approximation, as given for the higher-order discretization in Subsection 4.3, and hence we can skip the time splitting error.

The equation for the discretization is given by

$$\begin{aligned}
&\partial_t u_i \ + \ \nabla \cdot \mathbf{v}_i\ u_i \ = \ -\lambda_i u_i \ + \ \lambda_{i-1} u_{i-1}, \\
&i = 1, \ldots, m\ .
\end{aligned}$$

The velocity vector $\mathbf{v}$ is divided by R_i, and m is the number of concentrations. The initial conditions are given by $u_1^0 = u_1(x, 0)$, $u_i^0 = 0$ for $i = 2, \ldots, m$. The boundary conditions are trivial conditions, i.e. $u_i = 0$ for $i = 1, \ldots, m$.

We first calculate the maximal time step for cell j and for concentration i using the total outflow fluxes

$$\tau_{i,j} = \frac{V_j\ R_i}{\nu_j}\ , \quad \nu_j = \sum_{j \in out(i)} v_{i,j}\ .$$

We get the restricted time step with the local time steps of cells and their components

$$\tau^n \leq \min_{\substack{i=1,\ldots,m \\ j=1,\ldots,I}} \tau_{i,j}\ .$$

The velocity of the discrete equation is given by

$$v_{i,j} = \frac{1}{\tau_{i,j}}\ .$$

We calculate the analytical solution of the mass with equation (61) and (63) with

$$m^n_{i,jk,out} = m_{i,out}(a, b, \tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \,,$$
$$m^n_{i,j,rest} = m^n_{i,j}\ f(\tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \,,$$

where the parameters are $a = V_j R_i (c^n_{i,jk} - c^n_{i,jk'})$, $b = V_j R_i c^n_{i,jk'}$, and $m^n_{i,j} = V_j R_i u^n_i$. The linear impulse in the finite volume cell is $c^n_{i,jk'}$ for the concentration at the inflow and $c^n_{i,jk}$ for the concentration at the outflow boundary of cell j.

The discretization with the embedded analytical mass is calculated by

$$m^{n+1}_{i,j} - m^n_{i,rest} = -\sum_{k \in out(j)} \frac{v_{jk}}{\nu_j}\ m^n_{i,jk,out} + \sum_{l \in in(j)} \frac{v_{lj}}{\nu_l}\ m^n_{i,lj,out} \,,$$

where $\frac{v_{jk}}{\nu_j}$ is the retransformation of the total mass $m_{i,jk,out}$ into the partial mass $m_{i,jk}$. The mass in the next time step is $m^{n+1}_{i,j} = V_j\ c^{n+1}_i$, in the old time step it is the rest mass for the concentration i. The proof can be found in [11]. In the next section, we derive an analytical solution for the benchmark problem.

4.6 Analytical solutions of equilateral triangular initial conditions (the benchmark problem)

For our benchmark problem, we derive an exact solution for a triangular initial condition.

We could reset the initial condition for our equation (4) with a triangular impulse.

$$u_1(x,0) = c_0\ \tfrac{2}{\epsilon} \begin{cases} x\,, & x \in (0, \frac{\epsilon}{2}) \\ \epsilon - x\,, & x \in (\frac{\epsilon}{2}, \epsilon) \\ 0 & \text{otherwise} \end{cases} \,, \qquad (82)$$
$$u_i(x,0) = 0\,, \quad i = 2, \ldots, m \,,$$

where c_0 and ϵ are arbitrary positive constants. The initial conditions are transferred as follows:

$$\hat{u}_1(s,0) = c_0\ \frac{2}{\epsilon}\ \frac{(1 - \exp(-\frac{\epsilon}{2}s))^2}{s^2} \,. \qquad (83)$$

We reset this transformed initial condition for the initial condition in equation (9). We could retransform equation (13) for the transformed problem with the new initial condition and therefore get the following solution:

$$u_1(x,t) = c_0\ \frac{2}{\epsilon}\ \exp(-\lambda_1 t) \begin{cases} 0 & 0 \le x < v_1 t \\ x - v_1 t + b & v_1 t \le x < v_1 t + \frac{\epsilon}{2} \\ v_1 t + \epsilon - x & v_1 t \le x < v_1 t + \epsilon \\ 0 & v_1 t + \epsilon < x \end{cases} \,, \qquad (84)$$

$$u_i(x,t) = \Lambda_i\ \sum_{j=1}^{i} \exp(-\lambda_j t)\ \Lambda_{j,i} \sum_{\substack{k=1 \\ k \neq j}}^{i} A_{jk}\ \Lambda_{jk,i} \,, \qquad (85)$$

$$\text{with} \quad i = 2, \ldots, m \ ,$$

$$A_{jk} = \begin{cases} 0 & 0 \le x < v_j t \\ x - v_j t + \frac{1}{\lambda_{jk}}(-1 + \exp(-\lambda_{jk}(x - v_j t))) & v_j t \le x < v_j t + \frac{\epsilon}{2} \\ v_j t + \epsilon - x + \frac{1}{\lambda_{jk}}(\exp(-\lambda_{jk}(x - v_j t)) & \\ -2\exp(-\lambda_{jk}(x - (v_j t + \frac{\epsilon}{2}))) + 1) & v_j t + \frac{\epsilon}{2} < x < v_j t + \epsilon \\ \frac{1}{\lambda_{jk}}(\exp(-\lambda_{jk}(x - v_j t)) & \\ -2\exp(-\lambda_{jk}(x - (v_j t + \frac{\epsilon}{2}))) & \\ +\exp(-\lambda_{jk}(x - (v_j t + \epsilon)))) & v_j t + \frac{\epsilon}{2} < x < v_j t + \epsilon \end{cases} .$$

This analytical solution is used in the next section for the benchmark problem.

5 Numerical experiments

The numerical and analytical methods are programmed in our software package R^3T, described in [13], based on the software tool *ug* described in [2]. In this paper we will focus on the experiments; a description of the tools is presented in [11].

The numerical experiments are based on the comparison between the analytical and the numerical solutions. The results for the numerical solutions are achieved with the standard as well as with the modified method.

The standard method is based on an operator-splitting method using the higher-order finite volume discretization for the convection term and the analytical solution for the reaction term, cf. subsection 4.4. The modified method is achieved with higher-order finite volume methods for the convection and reaction term with respect to embedding the analytical solution, cf. subsection 4.5.

For the experiments we use the benchmark problem with triangular initial conditions. We calculate the solutions on a two-dimensional domain, for which we use a constant velocity field in the x-direction, given as $\mathbf{v} = (1.0, 0.0)^T$. The computation uses the convection-reaction equation and four components, given in the form

$$\begin{aligned} & R_i \, \partial_t u_i + \mathbf{v} \cdot \nabla u_i = -R_i \, \lambda_i \, u_i + R_{i-1} \, \lambda_{i-1} \, u_{i-1} \ , \\ & i = 1, \ldots, 4 \ , \end{aligned} \tag{86}$$

with the inflow and outflow boundary condition with $\mathbf{n} \cdot \mathbf{v} \, u_i = 0$. The initial conditions are given for the first component as

$$\begin{aligned} u_1(x,0) &= \begin{cases} x & 0 \le x \le 1 \\ 2 - x & 1 \le x \le 2 \\ 0 & \text{otherwise} \end{cases} \ , \\ u_i(x,0) &= 0 \ , \ i = 2, \ldots, 4 \ . \end{aligned} \tag{87}$$

The numerical solutions are compared with the analytical solutions by using the L_1-norm.

The L_1-norm is given as

$$E^i_{L_1,l} := \sum_{j=1,\ldots,N_l} V_{j,l} \; |u_{i,\mathrm{num}}(x_{j,l}, y_{j,l}, t^n) - u_i(x_{j,l}, y_{j,l}, t^n)|. \tag{88}$$

where N_l is the number of the nodes on grid level l, and $V_{j,l}$ is the volume of the j node on grid level l. The numerical solution is $u_{i,\mathrm{num}}(x_{j,l}, y_{j,l}, t^n)$ and $u_i(x_{j,l}, y_{j,l}, t^n)$ is the analytical solution of component i on the grid point j with the coordinates $(x_{j,l}, y_{j,l})$ and with time t^n.

The model domain is given by a rectangle of 8×1 units. The initial coarse grid is framed with quadratic unit elements. The computations are done with uniform refinements until the level 7 (131072 elements) is achieved.

The model time is given by $t = 0, \ldots, 6$. We compare the results at the ending time point $t = 6$. We apply the L_1-norm for the errors of the analytical and numerical solutions, but we can also use the L_∞-norm. The numerical convergence rate is computed as

$$\rho^i_{L_1,l+1} = (\log(E^i_{L_1,l+1}) - \log(E^i_{L_1,l}))/\log(0.5) \; , \tag{89}$$

where the levels are $l = 4, \ldots, 7$ and we assume the grid-width is divided in half on the next grid level, see [20].

We have selected different parameters for the reaction and retardation factors to present complex examples with different transport and reaction processes.

5.1 First experiment: ascending retardation factors

We use ascending parameters for the retardation factors. The retardation factors are given as $R_1 = 1, R_2 = 2, R_3 = 4, R_4 = 8$. The reaction factors are given as $\lambda_1 = 0.4, \lambda_2 = 0.3, \lambda_3 = 0.2, \lambda_4 = 0$.

The results for the standard method are presented in Table 1 .

l	$E^1_{L_1,l}$	$\rho^1_{L_1,l}$	$E^2_{L_1,l}$	$\rho^2_{L_1,l}$	$E^3_{L_1,l}$	$\rho^3_{L_1,l}$	$E^4_{L_1,l}$	$\rho^4_{L_1,l}$
4	0.0		$1.71\ 10^{-3}$		$1.04\ 10^{-3}$		$2.407\ 10^{-4}$	
5	0.0	∞	$8.61\ 10^{-4}$	0.989	$5.28\ 10^{-4}$	0.978	$1.22\ 10^{-4}$	0.98
6	0.0	∞	$4.29\ 10^{-4}$	1.005	$2.65\ 10^{-4}$	0.995	$6.13\ 10^{-5}$	0.993
7	0.0	∞	$2.14\ 10^{-4}$	1.003	$1.31\ 10^{-4}$	1.016	$3.07\ 10^{-5}$	0.997

Table 1. The L_1-error for ascending retardation factors computed with the standard method.

The results computed with the modified method are presented in Table 2. The first component in both methods has the same convergence rate. The computation is solved exactly and there are no differences between the methods, but for the next components we see differences in the convergence rates. The standard method tends to first-order because of the splitting error $O(\tau^n)$, whereas

l	$E^1_{L_1,l}$	$\rho^1_{L_1,l}$	$E^2_{L_1,l}$	$\rho^2_{L_1,l}$	$E^3_{L_1,l}$	$\rho^3_{L_1,l}$	$E^4_{L_1,l}$	$\rho^4_{L_1,l}$
4	0.0		$3.06\ 10^{-4}$		$3.91\ 10^{-5}$		$7.79\ 10^{-6}$	
5	0.0	∞	$8.03\ 10^{-5}$	1.95	$9.87\ 10^{-6}$	1.986	$2.15\ 10^{-6}$	1.89
6	0.0	∞	$2.007\ 10^{-5}$	2.00	$2.60\ 10^{-6}$	1.93	$5.81\ 10^{-7}$	1.89
7	0.0	∞	$4.36\ 10^{-6}$	2.21	$6.66\ 10^{-7}$	1.96	$1.51\ 10^{-7}$	1.94

Table 2. The L_1-error for ascending retardation factors computed with the modified method.

the modified method is a higher-order method because the convergence rates are > 1.

The results are visualized for the ending time point $t = 6$ in Figure 1. We see the first component, is weakly retarded and flows toward end of the interval. The next components are more retarded and also flow until the end of the interval, because of coupling with the other components. The last component is the most spread out because it has the strongest retardation.

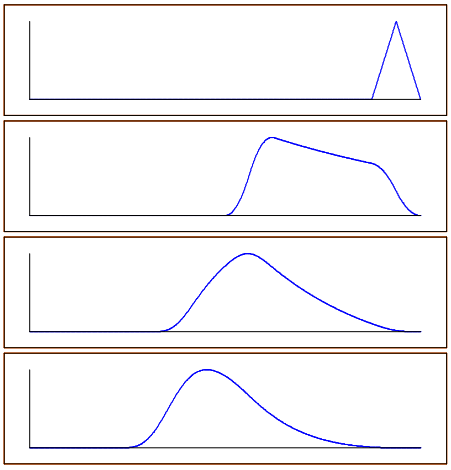

Fig. 1. Concentration for the four components with ascending retardation factors at time $t = 6$.

The next experiment is done with reciprocal parameters.

5.2 Second experiment: descending retardation factors

For the second example we use descending retardation factors to get another combination for different component-wise velocities.

The retardation factors are given as $R_1 = 8, R_2 = 4, R_3 = 2, R_4 = 1$. The reaction factors are given as $\lambda_1 = 0.3, \lambda_2 = 0.4, \lambda_3 = 0.5, \lambda_4 = 0$.

The results for the standard method are presented in Table 3.

l	$E^1_{L_1,l}$	$\rho^1_{L_1,l}$	$E^2_{L_1,l}$	$\rho^2_{L_1,l}$	$E^3_{L_1,l}$	$\rho^3_{L_1,l}$	$E^4_{L_1,l}$	$\rho^4_{L_1,l}$
4	$7.30\ 10^{-3}$		$5.55\ 10^{-3}$		$1.069\ 10^{-2}$		$2.502\ 10^{-2}$	
5	$2.57\ 10^{-3}$	1.58	$2.27\ 10^{-3}$	1.25	$5.16\ 10^{-3}$	1.051	$1.225\ 10^{-2}$	1.02
6	$9.36\ 10^{-4}$	1.53	$1.01\ 10^{-3}$	1.16	$2.52\ 10^{-3}$	1.033	$6.056\ 10^{-3}$	1.01
7	$3.52\ 10^{-4}$	1.45	$4.73\ 10^{-4}$	1.09	$1.24\ 10^{-3}$	1.023	$3.00\ 10^{-3}$	1.01

Table 3. The L_1-error for descending retardation factors computed with the standard method.

We also compute the results with the modified method. The results are presented in Table 4. We obtain only higher-order convergence for the first components, while the scalar equations do not have a splitting error, cf. [29]. But for the latter components, we obtain first-order convergence rates with the standard method, because of the splitting error in time. For the modified method we receive again the higher-order method with convergence rates > 1.

l	$E^1_{L_1,l}$	$\rho^1_{L_1,l}$	$E^2_{L_1,l}$	$\rho^2_{L_1,l}$	$E^3_{L_1,l}$	$\rho^3_{L_1,l}$	$E^3_{L_1,l}$	$\rho^4_{L_1,l}$
4	$7.30\ 10^{-3}$		$4.23\ 10^{-3}$		$1.43\ 10^{-3}$		$1.255\ 10^{-3}$	
5	$2.57\ 10^{-3}$	1.58	$1.14\ 10^{-3}$	1.89	$3.07\ 10^{-4}$	2.22	$2.82\ 10^{-4}$	2.15
6	$9.36\ 10^{-4}$	1.53	$2.49\ 10^{-4}$	2.24	$7.94\ 10^{-5}$	1.95	$6.81\ 10^{-5}$	2.05
7	$3.52\ 10^{-4}$	1.45	$5.82\ 10^{-5}$	2.11	$2.04\ 10^{-5}$	1.96	$1.68\ 10^{-5}$	2.02

Table 4. The L_1-error for descending retardation factors computed with the modified method.

The results for this experiment are visualized in the ending time point $t = 6$ in Figure 2. The first component is strongly retarded and flows only in the first part of the interval. The next components are more weakly retarded and flow further. Because of coupling between components, the next components are spread out and overlap with the previous components. The last component flows until the end of the interval and is the most spread out.

The experiments demonstrate the improvement of the modified methods for the higher components of the decay chain. The convergence rates are of higher-order and we receive these improved results in the same computing time.

We also get equal results for applications in higher dimensions and for complex problems. More applications are presented in paper [12].

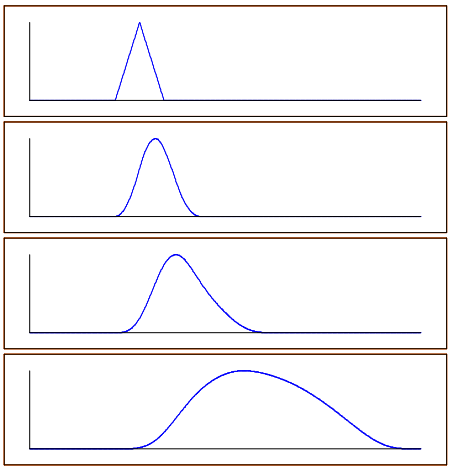

Fig. 2. Concentration for the four components with descending retardation factors at time $t = 6$.

6 Conclusions

We present a new discretization method based on the finite volume method with embedded analytical solutions. The modified method skips the splitting error in time and improves the order of the discretization. The analytical methods for the one-dimensional equations for a general case with different parameters are described and a generalization is proposed for enlargement for a reversible reaction and for equal parameters. The modified method with the embedded analytical solutions is presented. The advantages of this new method are considered in the applications. In future works, we will focus on special cases, e.g. nonlinearity, reversible reactions and diffusion terms.

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