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An Operator Splitting Approximation Combined With The SUPG Method For Transport Equations With Nonlinear Reaction Term

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Abstract: In this work, an operator splitting method is proposed in order to obtain a stable numerical solution for transport equation with non-linear reaction term. We split the transport equation into a reaction part and an advection diffusion part. The former one which becomes a nonlinear ordinary differential equation can be approximated by the simple higher order integrator or solved exactly. The later one is approximated by the Streamline-Upwind Petrov-Galerkin (SUPG) method combined with the generalized Euler time integration (θ-method). Numerical results that illustrate the good performance of this method are reported.

Keywords: Operator splitting, Stabilized finite element method, Nonlinear Reactive Transport equations, SUPG method.

1 Introduction

The mathematical models describing the transport phenomena are time dependent advection diffusion reaction equations. This kind of equation with linear or nonlinear reaction term is one for which approximate solution procedures continue to exhibit significant limitations for certain problems of physical interest. The most interesting cases are appear when advection is dominated. In this situation one is usually forced to choose between nonphysical oscillations or excessive diffusion.

In this paper we advocate an operator splitting method which is widely used to simulate the models come from environmental processes [Zlatev (1995);Geiser (2008);Levine, Pamuk, Sleeman and Nilsen-Hamilton (2001);Ewing (2002);Frolkovič and Geiser (2000)]. We split the transport equation into two unsteady subproblems. The main advantage of splitting is that each subproblem can be discretized separately by the convenient method independently of the other subproblem. According to our splitting strategy the first part is a first order nonlinear differ-

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ential equation without space derivatives and the second one is an unsteady linear advection diffusion problem. Although first problem can be solved exactly by using simple analytical technics or numerically by appropriate time integrator, the second one has some difficulties when advection is dominated. In this regime, it is well known that standard Galerkin finite element method yields poor approximation for steady or unsteady advection diffusion equations [Quarteroni and Valli (1996);Ross, Stynes and Tobiska (2008)]. In order to cope with this kind of problems, many stabilization techniques can be found in the literature. Among of them we focus on the most popular one the streamline-upwind Petrov/Galerkin (SUPG) method introduced by Brooks and Hughes [Brooks and Hughes (1982)] and analyzed by Johnson et al.[Johnson Navert and Pitkaranta (1984)]. A wide varierty of application of SUPG to many different problems can be found in the literature [Hughes, Franca and Balestra (1986);Brezzi and Douglas (1988); Franca and Frey (1992);Franca, Frey and Hughes (1992);Harari and Hughes (1994);Franca and Valentin (2000)]. We also use generalized Euler method (θ-method) for time discretization. It is known that SUPG method corresponds to adding a consistent term providing an additional diffusion in the streamline direction. The amount of such additional diffusion is tuned by a stabilized parameter τ which should be chosen in a suitable way. In order to ensure consistency, the discrete time derivative has to enter the stabilization which modifies the stability properties of the numerical scheme. It was shown by Bochev et al. [Bochev, Gunzburger and Shadid (2004)] that such implicit formulations always remain well posed regardless of the time step size. Their coercivity result however leads to suboptimal global estimates in time. Another important recent papers about SUPG type stabilization with θ method are [Burman (2010)] for pure advection equation, [Burman and Smith (2011)] for advection diffusion equation and [Lube and Weiss (1995);Frutos, Garcia-Archilla and Novo (2010);John and Novo (2011)] for advection diffusion reaction equation.

The layout of the paper is as follows. In section 2 we shortly review the SUPG strategy for time dependent advection diffusion equation with generalized Euler time integration. Section 3 introduces the transport problem under consideration and the operator splitting strategy is applied to decompose the main equation into two simpler ones. Finally Numerical results are presented in section 4.

2 Unsteady Advection-Diffusion Problem

Let Ω be an open bounded domain in $\mathbb{R}^d, (d = 1,2,3)$ with lipschitz continuous boundary $\partial\Omega$. We consider the initial boundary value problem:

$$\begin{aligned} u_t + Lu &= f \text{ in } \Omega_t := \Omega \times (0,T] \\ u &= 0 \text{ on } \partial\Omega \times [0,T] \\ u &= u^0 \text{ on } \Omega \times \{0\}. \end{aligned} \tag{1}$$

Here $u^0 \in L_2(\Omega)$ is given initial function and L is the elliptic operator, which depends on space variable, defined by

$$Lu := -\varepsilon \triangle u + \beta.\nabla u \tag{2}$$

where $\varepsilon > 0$ is a constant diffusion coefficient, β is divergence free advection field and $f \in L_2(0,T;L_2(\Omega))$ is given source function. Under these assumptions existence and uniqueness of the solution are guaranteed [Raviart and Thomas (1992)].
The weak formulation of the strong problem (1) reads:
For each $t \in (0,T]$ find $u(t) \in H_0^1(\Omega)$ satisfying

$$\begin{aligned} \frac{d}{dt}(u(t),v) + a(u(t),v) &= (f(t),v)\ \forall v \in H_0^1(\Omega), \\ u(0) &= u^0. \end{aligned} \tag{3}$$

where the bilinear form $a : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ is given by

$$a(u,v) := \varepsilon(\nabla u, \nabla v) + (\beta.\nabla u, v). \tag{4}$$

As usual, $(.,.)_{\mathfrak{D}}$ denotes the inner product in $L^2(\mathfrak{D})$, where $\mathfrak{D}$ is an open subset of Ω. To simplify the notation, for the case $D = \Omega$, we just write $(.,.)$. Let $\mathfrak{T}_h$ be a standard partition of Ω into elements K and let $V_h \subset H_0^1(\Omega)$ be the corresponding finite element space of piecewise linear polynomials:

$$V_h := \{v_h \in H_0^1(\Omega) \cap C^0(\Omega) : v_h|_K \text{ is linear polynomial } \forall K \in \mathfrak{T}_h\}$$

A first step towards the approximation of the solution (3) entails the discretization of the space variable only. This leads to system of ordinary differential equation, whose solution $u_h(t)$ is an approximation of the exact solution for each $t \in [0,T]$. Then the semi-discrete Galerkin approximation reads as follows:
For each $t \in (0,T]$ find $u_h(t) \in V_h \subset H_0^1(\Omega)$ that satisfies

$$\begin{aligned} \frac{d}{dt}(u_h(t),v_h) + a(u_h(t),v_h) &= (f(t),v_h)\ \forall v_h \in V_h, \\ u_h(0) &= u_h^0. \end{aligned} \tag{5}$$

Here we choose $u_h^0 \in V_h$ as the standard interpolation of the initial datum u^0. It is well known that steady or unsteady advection-diffusion equation may exhibit sharp layers when the advection term dominates the diffusion one. In this case, using the standard Galerkin finite element approach, especially using low order polynomial spaces, with a partition scale which is too big to compute the layers, produces nonphysical oscillations in large part of the domain. To accurately resolve the layers, the mesh size must be of the same size as the ratio between diffusion and the modulus of the advection term. However, that requires an extremely small mesh size, which is not affordable in practical computations in many problems. Since we are interested in finding a finite element discretization for (3) that is stable and coarse mesh accurate for all ε and β, we use the SUPG spatial stabilization [Brooks and Hughes (1982)] such that:
For each $t \in (0,T]$ find $u_h(t) \in V_h \subset H_0^1(\Omega)$ that satisfies

$$\begin{aligned} \frac{d}{dt}(u_h(t),v_h) + a(u_h(t),v_h) &+ \sum_{K\in\mathfrak{T}_h} \tau_K(\frac{du_h(t)}{dt} + \beta.\nabla u_h(t) - f(t), \beta.\nabla v_h)_K \\ &= (f(t),v_h) \ \forall v_h \in V_h, \\ u_h(0) &= u_h^0. \end{aligned} \tag{6}$$

The stability parameter τ_K we will be using accommodates usage of higher order interpolations and it can be understood a posteriori based on a priori error analysis. The formula are as follows (see [Franca, Frey and Hughes (1992);Harari and Hughes (1992)]):

$$\tau_K = \begin{cases} \dfrac{h_K}{6||\beta||}, & Pe_K := \dfrac{||\beta||h_K}{6\varepsilon} > 1 \\ \dfrac{h_K^2}{12\varepsilon}, & \text{otherwise} \end{cases} \tag{7}$$

where h_K denotes the local mesh size and Pe_K denotes the local Peclet number which characterize the approximation as advection or diffusion dominated at element level.

In order to obtain a full discretization of (3), we consider a uniform partition for the time interval t and define

$$t_n := nk \ , \ n = 0,1,..,N \text{ where } k = T/N. \tag{8}$$

We replace the time derivative by means of suitable difference quotients, thus constructing a sequence u_h^n that approximates the exact solution at time t^n i.e. $u_h^n \approx u(t^n)$. For simplicity we restrict ourselves to the generalized trapezoidal rule

(θ-method). Applying the θ-scheme to the semi discrete equation (6), we obtain the following fully discrete problem: Find $u_h^n \in V_h$ such that for all $v_h \in V_h$

$$\left(\frac{u_h^{n+1}-u_h^n}{k}, v_h\right) + a\left(u_h^{n+\theta}, v_h\right) + \sum_{K\in\mathfrak{T}_h} \tau_K \left(\frac{u_h^{n+1}-u_h^n}{k} + \beta.\nabla u_h^{n+\theta} - f^{n+\theta}, \beta.\nabla v_h\right)_K = \left(f^{n+\theta}, v_h\right). \quad (9)$$

Here we have used some compact notation as $f^{n+\theta} = (1-\theta)f(t^n) + \theta f(t^{n+1})$ and $u_h^{n+\theta} = (1-\theta)u_h^n + \theta u_h^{n+1}$ where $\theta \in [0,1]$ is a parameter. When $\theta = 0$ or $\theta = 1$, this scheme is called forward Euler or backward Euler method, respectively. For numerical simulations, we prefer to choose backward Euler scheme ($\theta = 1$) which is first order accurate and A-stable [Lambert (1991)]. From the analysis in [Bochev, Gunzburger and Shadid (2004)] we know that implicit time integration with SUPG discretization in space improve the phase accuracy for advection dominated flows. Therefore we can safely use the scheme coupling SUPG in space and implicit Euler in time for unsteady equation.

3 Transport Problem with Nonlinear Reaction

In this section we consider a model equation for simulating the transport and decay of particles in a fluid:

$$\begin{aligned} u_t + Lu &= R(u) + f \text{ in } \Omega_t := \Omega \times (0,T] \\ u &= 0 \text{ on } \partial\Omega \times [0,T] \\ u &= u^0 \text{ on } \Omega \times \{0\} \end{aligned} \quad (10)$$

where elliptic operator L, source function f and initial datum u^0 are defined in previous section and R(u) is a nonlinear reaction term comes from the following models:

- Radioactive decay model: $R(u) = -au$.
- Logistic model : $R(u) = au - bu^2$.
- Bio-remediation model : $R(u) = \dfrac{au}{u+b}$.

Here a and b are nonnegative real numbers for each model. In order to simplify the notation, let us define

$$L_f(u) := f - Lu$$

Then the equation (10) can be read

$$u_t = L_f(u) + R(u)$$

An efficient approach for finding the approximate solution of (10) is based on an operator splitting strategy. The principle of this procedure is starting from u_h^n, an approximation $u(t^n,.)$, construct u_h^{n+1} through two or more intermediate values, each one obtained by solving a boundary value problem related to only one of the separating operators. In the literature authors generally prefer to separate diffusion from advection [Quarteroni and Valli (1996);Geiser, Erwing and Liu (2005)]. Differently to this prevailing opinion we separate the non-linear reaction term from advection diffusion term such that

$$w_t = R(w). \tag{11}$$
$$z_t = L_f(z) \tag{12}$$

Since R and L_f are not commute operator except for radioctive decay model, we obtain a splitting error first order ($O(k)$). On the other hand our splitting has two important advantages that we can apply stabilized finite element method SUPG with backward Euler time stepping to (12), which is done in previous section, and exact solution of (11) can be easily obtained.

$$\begin{aligned} w_t &= R(w) \text{ in } \Omega_t := \Omega \times (0,T) \\ w &= \phi \text{ on } \Omega \times \{0\} \end{aligned} \tag{13}$$

Exact solution of the equation (13) can be given for each reaction terms described above such that

- Radioactive decay model : $w(x,t) = e^{-at}\phi(x)$
- Logistic model: $w(x,t) = \dfrac{a\phi(x)}{b\phi(x)(1-e^{-at}) + ae^{-at}}$
- Bio-remediation model : $w(x,t) + bln|w(x,t)| = at + \phi(x) + bln|\phi(x)|$

For more complex cases, one may use an appropriate time integrator for instance generalized Euler or Runge Kutta (RK) methods instead of their exact expressions.

We also use the two step Yanenko splitting strategy (see Fig. 1) which is first order accurate and unconditionally stable if the discrete counterparts of the differential operators are non-negative definite matrices [Marchuk (1990)].

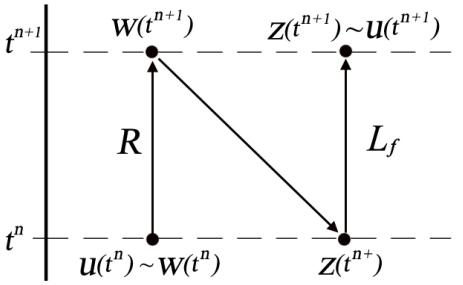

Figure 1: Two step Yanenko splitting scheme.

More formal description of two step Yanenko splitting method can be given in the following algorithm. Starting with $z(t^0) = u^0$, then two subproblems are sequentially solved on the sub-intervals $(t^n, t^{n+1}]$, $n = 0, ..., N-1$:
Given $z(t^n)$ find $w : \Omega \times (t^n, t^{n+1}] \to \mathbb{R}$ such that

$$\begin{aligned} w_t &= R(w) \text{ in } \Omega \times (t^n, t^{n+1}] \\ w(t^n) &= z(t^n) \text{ on } \Omega. \end{aligned} \tag{14}$$

Find $z : \Omega \times (t^n, t^{n+1}] \to \mathbb{R}$ such that

$$\begin{aligned} z_t &= L_f(z) \text{ in } \Omega \times (t^n, t^{n+1}] \\ z &= 0 \text{ on } \partial\Omega \times [t^n, t^{n+1}] \\ z(t^{n+}) &= w(t^{n+1}) \text{ on } \Omega. \end{aligned} \tag{15}$$

This two step splitting algorithm presents $z(t^n)$, $n = 1, ..., N$ which is an approximation of $u(t^n)$.

4 Numerical Experiments

We firstly test our method for the following one-dimensional transport problems:

$$\begin{aligned} u_t - 0.0001u_{xx} + u_x &= R(u) + 1 \text{ in } \Omega_t := (0,1) \times (0,2] \\ u(0,t) = u(1,t) &= 0 \text{ for } t \in [0,2] \\ u(x,0) &= 0 \text{ for } x \in (0,1). \end{aligned} \tag{16}$$

where the reaction term is chosen as follows:

- Radioactive decay model : $R(u) = -15u$.

- Logistic model : $R(u) = 15u - u^2$.
- Bio-remediation model : $R(u) = \dfrac{15u}{u+1}$.

For all numerical simulation $N = 400$ uniform time steps are used and space discretization $\mathfrak{T}_h$ of $\Omega = (0,1)$ is made by 20 quasi-uniform subintervals. For all numerical methods we obtain a sequence of continuous piecewise linear approximation u_h^n $(n = 1,2,...,400)$ then we only compare the final time results obtained by different schemes. In Fig. (2) and Fig (3)(left), red curve (labeled with splitting with SUPG) and blue curve (labeled with standard splitting) were obtained by our algorithm (14)-(15) and the algorithm proposed in [Geiser, Erwing and Liu (2005)], respectively. The reference approximations (full black curve) were computed with the standard Galerkin method on a very fine mesh and with sufficiently small time steps. Dotted black curve in the Fig. 2(left) also illustrates the result obtained by the standard Galerkin method on the coarse mesh for radioactive decay model.

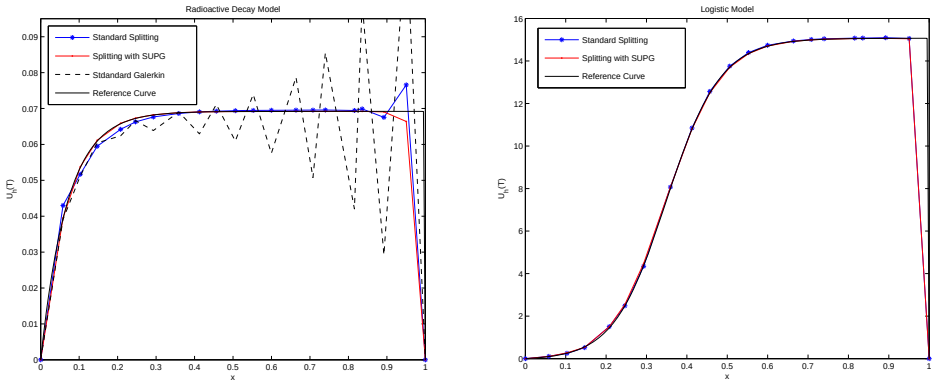

Figure 2: Numeric simulations for radioactive decay model (left) and logistic model (right).

The convergence plot in Fig. 3 (right) is presented by using 400-450-500-550-600-650 time steps for the radioactive decay test model:

$$\begin{aligned} u_t - 0.01u_{xx} + u_x &= -15u \text{ in } \Omega_t := (0,1)\times(0,2] \\ u(0,t) = u(1,t) &= 0 \text{ for } t \in [0,2] \\ u(x,0) &= \exp(50x)\sin(\pi x). \end{aligned} \tag{17}$$

In this case exact solution of the problem (17) can be written:

$$u(x,t) = \exp(50x - 40t - 0.01\pi^2 t)\sin(\pi x).$$

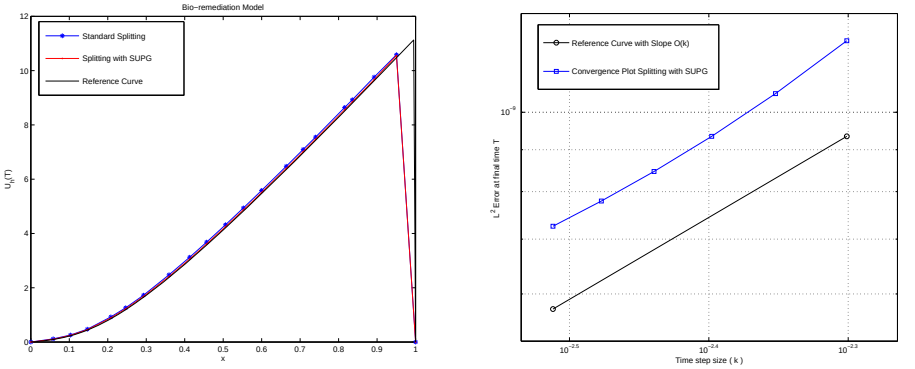

Figure 3: Numeric simulation for bio-remediation model (left) and error rate for the radioactive decay model (right).

As we see in Fig. 3 (right), our splitting algorithm presents first order convergence with respect to the time step size.

Finally we illustrate the numerical performance of our splitting strategy for two dimensional problems:

$$\begin{aligned} u_t - 0.0001\triangle u + (1,1).\nabla u &= R(u) \text{ in } \Omega_t := \Omega \times (0,T] \\ u &= 0 \text{ on } \partial\Omega \times [0,T] \\ u &= u^0 \text{ on } \Omega \times \{0\} \end{aligned} \tag{18}$$

where the reaction term is chosen as follows:

- Radioactive decay model : $R(u) = -3u$.
- Logistic model : $R(u) = 3u - u^2$.
- Bio-remediation model : $R(u) = \dfrac{3u}{u+1}$

and space discretization $\mathfrak{T}_h$ of $\Omega = (0,1)^2$ is made by 800 quasi-uniform triangles described in Fig. 4 (left). We choose final time $T = 1/2$ and fixed time step size $k = T/400$. We also choose a discrete initial data whose form is square prism of height 1 such that

$$u_0(x,y) = \begin{cases} 1, & (x,y) \in [\frac{3}{16}, \frac{6}{16}]^2 \\ 0, & \text{otherwise} \end{cases} \tag{19}$$

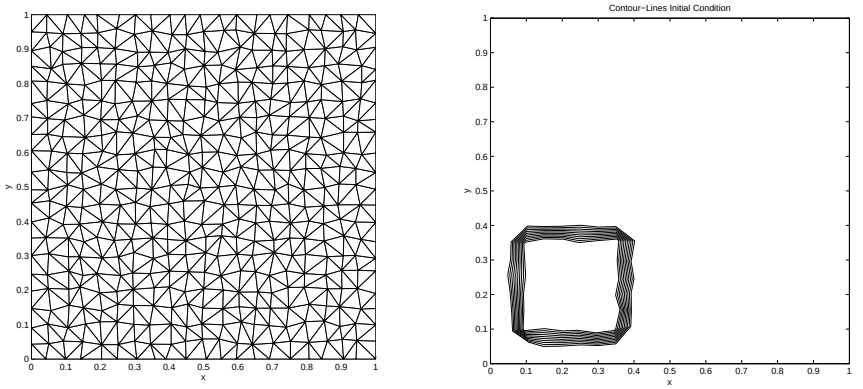

Figure 4: Quasi-uniform mesh (left) and contour-lines of the initial data (right).

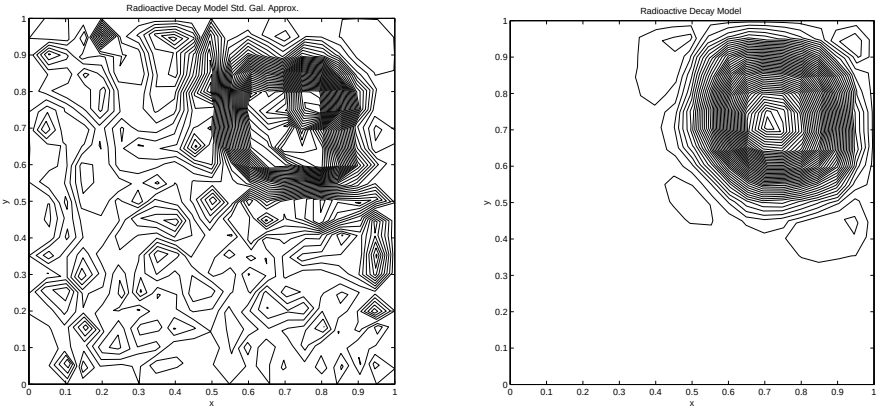

Figure 5: Contour-lines of Galerkin approximation (left) and our splitting algorithm (right) for the radioactive decay model at the final time.

The contour-lines of the interpolant of the initial data is shown in Fig. 4(right). We also compare the final time results obtained by the standard Galerkin approximation and our splitting algorithm in Fig. 5. As we see in this figure, although the Galerkin approximation is completely contaminated by spurious oscillations all over the whole domain Ω, our splitting strategy provides oscillation-free approximations. We also give the satisfactory results of our splitting algorithm for the

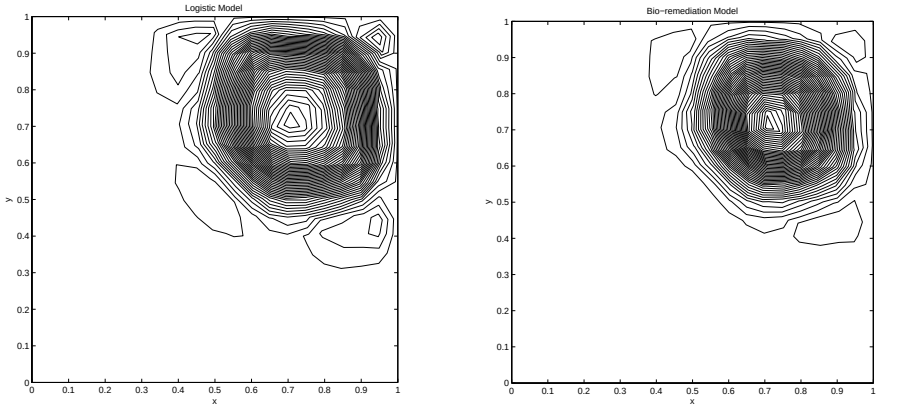

Figure 6: Contour-lines of our operator splitting approximation for the logistic (left) and bio-remediation (right) models at the final time.

logistic and bio-remediation model in Fig. 6.

5 Conclusion

This paper presents an operator splitting method for solution of transport problems with non-linear reaction term. Numerical results indicate that this splitting strategy can be considered a reliable and accurate method. Extension of this models are reactive-transport of multiple species which are described by set of coupled equations [Celia, Kindred and Herrera (1989)]. We believe that proposed method can be adapted these more realistic problems.

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