# Contaminant Transport in Porous Media by a Finite Volume Method

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**Abstract**

A cell-centered Finite-Volume method is proposed to solve the unsteady reactive diffusive transport of a contaminant in porous media. Two theoretical properties of the analitical solution, namely non-negativity and maximum principle, are mentioned and their implication on the approximation method are discussed.

**keywords.** Contaminant Transport, Finite Volumes, M-matrices.

## 1. Introduction

A cell-centered Finite-Volume (FV) scheme for the transport of contaminant in porous media is presented. The contaminant is advected by the groundwater bulk flow, it is diffused in the porous media and can react. In this paper we discuss the derivation of the scheme and we mention two analytical properties of the continuous problem, namely the non-negativity of the solution and the existence of a global maximum principle, that are ensured in a discrete form by the FV approximation.

The paper is organized as follows. In section 2 we show the governing equations and we mention the analytical properties that we want to focus on. In section 3 we discuss the FV framework. In section 4 we illustrate the properties of the reconstruction algorithm required to attain second-order accuracy. Finally, in section 5 we present the conclusions.

## 2. Reactive and Diffusive Transport

Let us indicate by $\Omega$ the computational domain where the model equation is defined. Mathematically, $\Omega$ is a connected polygonal domain in $\mathbb{R}^2$ defined by a closed (1-D) surface $\partial\Omega$.

We assume that $\Omega$ is homogeneously filled by a porous medium where the bulk flow takes place. The governing equation of the phenomenon we are interested in reads as

$$(RC)_t + \nabla \cdot (\mathbf{V}C - D\nabla C) = S \quad \text{in} \quad \mathbb{R}^+ \times \Omega. \tag{1}$$

Equation (1) describes the time-dependent reaction-advection-diffusion of a contaminant whose spatial concentration distribution is denoted by $C(t, \mathbf{x})$. The contaminant is passively advected by $\mathbf{V}(t, \mathbf{x})$, which is an assigned convection field; $D(t, \mathbf{x})$ is the diffusion tensor, $R(t, \mathbf{x})$ is the retardation factor, and $S(t, \mathbf{x})$ is the contaminant production/consumption source term [5].

This model problem is completed by furnishing an initial solution, that is the spatial distribution of the contaminant at time $t = 0$ within the domain $\Omega$,

$$C(0, \mathbf{x}) = C_0(\mathbf{x}), \qquad \mathbf{x} \in \Omega,$$

and a set of suitable boundary conditions that can be either of Dirichlet-type or of Neumann type. The boundary $\partial\Omega$ is usually the union of two non-overlapping and possibly empty subsets, $\Gamma_D$ and $\Gamma_N$, where respectively Dirichlet and Neumann type conditions are specified: $\partial\Omega = \Gamma_D \cup \Gamma_N$. Formally, the boundary conditions are expressed by using two smooth functions, $\mathsf{g_d}$ and $\mathsf{g_n}$, such that we have

$$\begin{aligned} &\text{Dirichlet :} \quad && C && = \mathsf{g_d} \quad \text{on} \quad \mathbb{R}^+ \times \Gamma_D, \\ &\text{Neumann :} \quad && D\nabla C \cdot \mathbf{n} && = \mathsf{g_n} \quad \text{on} \quad \mathbb{R}^+ \times \Gamma_N. \end{aligned} \tag{2}$$

Furthermore, the reactive source term, which can take into account both production of contaminants, due for example to pollution leakage, and consumption, due for example to a remediation intervention, takes the following rather general form,

$$S(t, \mathbf{x}, C) = -A(t, \mathbf{x}, C)C(t, \mathbf{x}) + B(t, \mathbf{x}, C),$$

where $A(t, \mathbf{x}, C)$ and $B(t, \mathbf{x}, C)$ are two smooth and non-negative functions.

### 2.1. Basic Analytical Results

Under some general assumptions on the initial contaminant distribution and the boundary conditions imposed on the model problem, it is possible to prove the non-negativity of the contaminant concentration and a global maximum principle [6]. This is stated by the two following propositions.

**Proposition 1 (Non-Negativity)**

$$\begin{aligned} &\textit{If} \quad C_0(\mathbf{x}) \geq 0, \quad \mathsf{g_d}(t, \mathbf{x}) \geq 0, \quad \textit{and} \quad \mathsf{g_n}(t, \mathbf{x}) \geq 0 \\ &\textit{then} \qquad 0 \leq C(t, \mathbf{x}) \qquad \textit{for } t > 0, \ \textit{and } \mathbf{x} \in \Omega. \end{aligned}$$

**Proposition 2 (Global Maximum Principle)**

$$\begin{aligned} &\textit{If} \qquad C_0(\mathbf{x}) \geq 0, \quad \mathsf{g_d}(t, \mathbf{x}) \geq 0, \quad \mathsf{g_n}(t, \mathbf{x}) = 0, \quad \textit{and} \quad S = 0, \\ &\textit{then} \qquad 0 \leq C(t, \mathbf{x}) \leq M(t) \qquad \textit{for } t > 0, \ \textit{and } \mathbf{x} \in \Omega, \\ &\textit{where} \quad M(t) = \max \left\{ \sup_{\mathbf{x} \in \Omega} C_0(\mathbf{x}), \ \sup_{\tau \in (0,t)} \sup_{\mathbf{x} \in \Gamma^D} \mathsf{g_d}(\tau, \mathbf{x}) \right\}. \end{aligned}$$

In the rest of the paper we illustrate the design of a cell-centered FV method that ensures a discrete version of these properties. Basically, the discrete version of Proposition 1 guarantees that the numerical approximation of $C$ is a non-negative field, while the discrete version of Proposition 2 guarantees that the numerical approximation of $C$ satisfies a stability constraint.

## 3. The Finite Volume Formulation

The design of our FV method starts as usual by reformulating in an integral form the model problem defined by equations (1) and (2) on a set of closed and non-overlapping control volumes $\mathsf{T}_i \in \mathcal{T}_h$, where $\mathcal{T}_h$ is a conformal triangulation of $\Omega$ [4]. Integrating equation (1) over $\mathsf{T}_i$, applying the Gauss divergence theorem and imposing when required the boundary conditions given in (2), we have

$$\begin{aligned} &\frac{\partial}{\partial t}\int_{\mathsf{T}_i} R(\cdot,\mathbf{x})C(\cdot,\mathbf{x})\,d\mathbf{x} + \sum_{j\in\mathcal{T}_h(i)}\int_{\mathsf{e}_{ij}}\Big[C(\cdot,\mathbf{x})\mathbf{V}(\cdot,\mathbf{x}) - D(\cdot,\mathbf{x})\nabla C(\cdot,\mathbf{x})\Big]\cdot\mathbf{n}_{ij}\,d\ell + \\ &\sum_{j'\in\mathcal{T}_h^d(i)}\int_{\mathsf{e}_{ij}} \mathsf{g_d}(\cdot,\mathbf{x})\mathbf{V}(\cdot,\mathbf{x})\cdot\mathbf{n}_{ij}\,d\ell - \sum_{j'\in\mathcal{T}_h^n(i)}\int_{\mathsf{e}_{ij}} \mathsf{g_n}(\cdot,\mathbf{x})\cdot\mathbf{n}_{ij}\,d\ell = \\ &\int_{\mathsf{T}_i}\Big[-A(C(\cdot,\mathbf{x}))C(\cdot,\mathbf{x}) + B(C(\cdot,\mathbf{x}))\Big]\,d\mathbf{x}, \qquad \text{for every } \mathsf{T}_i\in\mathcal{T}_h. \end{aligned} \tag{3}$$

In (3) $\mathcal{T}_h(i)$ is the index set of volumes adjacent to $\mathsf{T}_i$, $\mathsf{e}_{ij}$ is the edge shared by $\mathsf{T}_i$ and $\mathsf{T}_j$, i.e. $\mathsf{e}_{ij} = \mathsf{T}_i \cap \mathsf{T}_j$, and $\mathcal{T}_h^d(i)$ and $\mathcal{T}_h^n(i)$ the index set of the edges of $\mathsf{T}_i$ located on the domain boundary, i.e. $\mathsf{e}_{ij} = \mathsf{T}_i \cap \partial\Omega$. The symbol $\mathbf{n}_{ij}$ denotes the vector that is normal to the edge $\mathsf{e}_{ij}$ and oriented from $\mathsf{T}_i$ to $\mathsf{T}_j$ when the edge is internal, or outward-directed when the edge is on the boundary.

The Finite Volume method is formulated on each volumes $\mathsf{T}_i \in \mathcal{T}_h$ by the equation

$$|\mathsf{T}_i|\,\frac{dr_i c_i}{dt} + \sum_{j\in\mathcal{T}_h(i)}\Big[\underbrace{\mathrm{G}_{ij}(\mathbf{c})}_{\text{convection}} + \underbrace{\mathrm{H}_{ij}(\mathbf{c})}_{\text{diffusion}}\Big] + \sum_{j\in\mathcal{T}_h'(i)}\underbrace{\mathrm{F}_{ij'}(\mathbf{c})}_{\text{boundary}} = \underbrace{S_i(\mathbf{c})}_{\text{source}}, \tag{4}$$

where we indicate the numerical flux integral terms corresponding to the ones in (3). In (4) $r_i$ is the $\mathsf{T}_i$ cell-average of the retardation factor $R$.

We denote the piecewise-linear FV approximation of $C$ by $\widetilde{c}(\cdot,\mathbf{x})$. The restriction of $\widetilde{c}(\cdot,\mathbf{x})$ to the cell $\mathsf{T}_i \in \mathcal{T}_h$ is

$$\widetilde{c_i}(\cdot,\mathbf{x}) = c_i + \widetilde{\mathcal{G}_i}(\mathbf{c})\cdot(\mathbf{x}-\mathbf{x}_i), \qquad \mathbf{x}\in\mathsf{T}_i, \tag{5}$$

where $c_i$ is the approximation of the cell average of $C$ within $\mathsf{T}_i$,

$$c_i \approx \frac{1}{|\mathsf{T}_i|}\int_{\mathsf{T}_i} C(\cdot,\mathbf{x})\,d\mathbf{x},$$

and $\widetilde{\mathcal{G}_i}$ is the approximation of the gradient of the solution within the same cell. The gradient approximation is calculated by using the FV cell average in $\mathsf{T}_i$ and the ones within the surrounding cells and a special limited reconstruction algorithms. The limiter is introduced to control the numerical oscillations that can appear in the approximation process. Major details about these issues are described in the next section.

### 3.1. Least-Square Vertex Reconstruction

The calculation of the integrals of the convective and diffusive numerical fluxes in (4) involves both *cell*-centered and *edge*-centered estimates of the solution gradient. The formers were introduced in (5) and are denoted by the symbol $\widetilde{\mathcal{G}}_i$, while the latters by the symbol $\widetilde{\mathcal{G}}_{ij}(\mathbf{c})$. The first step in the calculation of these quantities consists in the recovery of the solution approximation at the mesh vertices from the cell-average solution values. To this purpose, we consider a linear Least-Square (LS) approximation of the set of triplets

$$\left\{ \Big( x_i,\ y_i,\ c_i \Big),\ i \in \mathcal{T}_h(\alpha) \right\},$$

where $\mathcal{T}_h(\alpha)$ is the set of cells sharing the vertex $\alpha$. That is, we seek for the following representation of the solution at each vertex $\alpha$ with coordinates $(x_\alpha, y_\alpha)$

$$c_\alpha = a + bx_\alpha + cy_\alpha, \tag{6}$$

where $a$, $b$ and $c$ are the minimizers of

$$E(a,b,c) = \sum_{i \in \mathcal{T}_h(\alpha)} \lambda_{\alpha i} \left( a + bx_i + cy_i - c_i \right)^2,$$

and $\{\lambda_{\alpha i}\}$ is an assigned set of normalized non-negative weights. After some algebraic manipulations equation (6) takes the form

$$c_\alpha = \sum_{j \in \mathcal{V}_h(\alpha)} w_{\alpha j}\, c_j,$$

where

$$\begin{aligned} &w_{\alpha j} = \lambda_{\alpha j} \left( 1 + (\mathbf{x}_\alpha - \mathbf{x}_\alpha^G)^T \mathbf{S}_\alpha^{-1} (\mathbf{x}_j - \mathbf{x}_\alpha^G) \right), \\ &\mathbf{x}_\alpha^G = \sum_{j \in \mathcal{T}_h(\alpha)} \lambda_{\alpha j} \mathbf{x}_j, \qquad \text{and} \qquad \mathbf{S}_\alpha = \sum_{j \in \mathcal{T}_h(\alpha)} \lambda_{\alpha j} (\mathbf{x}_j - \mathbf{x}_\alpha^G)(\mathbf{x}_j - \mathbf{x}_\alpha^G)^T. \end{aligned} \tag{7}$$

The relation between the set of coefficients $w_{\alpha j}$ and $\lambda_{\alpha i}$ is expressed by the equations (7). A possible and usual choice for the latters is

$$\lambda_{\alpha i} = \frac{|\mathsf{T}_i|}{\sum_{k \in \mathcal{T}_h(\alpha)} |\mathsf{T}_k|},$$

but the weights $w_{\alpha j}$ can be negative or take very large values when the mesh cells are stretched [7]. However, it is possible to show that there exists $\lambda_{\alpha i}$ such that $w_{\alpha j}$ are strictly positive weights [1].

## 3.2. Limited Gradient Reconstruction and Discretization of the Advection Term

The piecewise-constant gradient $\widetilde{\mathcal{G}}_i(\mathbf{c})$ within the cell $\mathsf{T}_i$ is reconstructed by using the formula

$$\widetilde{\mathcal{G}}_i(\mathbf{c}) = \ell_i \frac{1}{2\,|\mathsf{T}_i|}\mathbf{R}\Big[c_\alpha(\mathbf{x}_\beta - \mathbf{x}_\gamma) + c_\beta(\mathbf{x}_\gamma - \mathbf{x}_\alpha) + c_\gamma(\mathbf{x}_\alpha - \mathbf{x}_\beta)\Big].$$

This gradient is such that the vector $(\widetilde{\mathcal{G}}_i(\mathbf{c}), 1)$ is orthogonal to the plane for the 3-D vectors $(\mathbf{x}_\alpha, c_\alpha)$, $(\mathbf{x}_\beta, c_\beta)$ and $(\mathbf{x}_\gamma, c_\gamma)$.

The scalar limiting factor $\ell_i$ is the largest real number in $[0,1]$ such that

$$
\begin{array}{lll}
(i) & \min\{c_i, c_j\} \leq \widetilde{c}_i(\cdot, \mathbf{x}_{ij}) \leq \max\{c_i, c_j\} & \mathsf{e}_{ij} \in \mathcal{E}_h^I \\
(ii) & \min\{c_i, \mathsf{gd}_{ij'}\} \leq \widetilde{c}_i(\cdot, \mathbf{x}_{ij'}) \leq \max\{c_i, \mathsf{gd}_{ij'}\} & \mathsf{e}_{ij'} \in \mathcal{E}_h^D \\
(iii) & \Big(\widetilde{\mathcal{G}}_i(\mathbf{c}) \cdot \mathbf{n}_{ij}\Big) \cdot \mathsf{gn}_{ij} \geq 0 & \\
 & \Big|d_{ij}\widetilde{\mathcal{G}}_i(\mathbf{c}) \cdot \mathbf{n}_{ij}\Big| \leq |\mathsf{gn}_{ij}| & \mathsf{e}_{ij'} \in \mathcal{E}_h^N, \\
 & \text{and} \qquad d_{ij} = \displaystyle\int_{\mathsf{e}_{ij}} D(\cdot, \mathbf{x})\, d\ell. &
\end{array}
$$

The advection term in equation (3) is discretized by using a standard upwind technique. We have

$$
\begin{aligned}
\mathrm{G}_{ij}(C) &= \nu_{ij}^{+}\widetilde{c}_i(\cdot, \mathbf{x}_{ij}) + \nu_{ij}^{-}\widetilde{c}_j(\cdot, \mathbf{x}_{ij}) = \nu_{ij}^{+}\widetilde{c}_i(\cdot, \mathbf{x}_{ij}) - \nu_{ji}^{+}\widetilde{c}_j(\cdot, \mathbf{x}_{ij}), \\
&\approx \int_{\mathsf{e}_{ij}} C(\cdot, \mathbf{x})\mathbf{V}(\cdot, \mathbf{x}) \cdot \mathbf{n}_{ij}\, d\ell, \qquad j \in \mathcal{T}_h(i),
\end{aligned}
\tag{8}
$$

where we introduced the edge-average integral of the velocity field and its upwind value

$$\nu_{ij} = \int_{\mathsf{e}_{ij}} \mathbf{V}(\cdot, \mathbf{x}) \cdot \mathbf{n}_{ij}\, d\ell, \qquad \nu_{ij}^{\pm} = \frac{\nu_{ij} \pm |\nu_{ij}|}{2},$$

and exploited the fact that $\nu_{ij}^{-} = -\nu_{ji}^{+}$.

## 3.3. Edge Limited Gradient Reconstruction and Discretization of the Diffusive Term

The gradient reconstruction at each internal edge proceeds throughout the following three steps:

(i) compute $\mathcal{G}_{ij}(\mathbf{c}) = \dfrac{3}{2\,|\mathsf{T}_i|}\mathbf{R}\left[(\mathbf{x}_\beta - \mathbf{x}_i)(c_\alpha - c_i) - (\mathbf{x}_\alpha - \mathbf{x}_i)(c_\beta - c_i)\right]$,
which is such that the vector $(\mathcal{G}_{ij}(\mathbf{c}), 1)$ is orthogonal to the plane for the 3-D points $(\mathbf{x}_k, c_k)$ with $k = i$, $\alpha$, $\beta$;

(ii) compute $\mathcal{G}_{ji}(\mathbf{c}) = \dfrac{3}{2\,|\mathsf{T}_j|}\mathbf{R}\left[(\mathbf{x}_\alpha - \mathbf{x}_j)(c_\beta - c_j) - (\mathbf{x}_\beta - \mathbf{x}_j)(c_\alpha - c_j)\right]$,
which is such that the vector $(\mathcal{G}_{ij}(\mathbf{c}), 1)$ is orthogonal to the plane for the 3-D points $(\mathbf{x}_k, c_k)$ with $k = j$, $\alpha$, $\beta$;

(iii) compute the non-linear average between $\mathcal{G}_{ij}(\mathbf{c})$ and $\mathcal{G}_{ji}(\mathbf{c})$

$$\begin{aligned} \widetilde{\mathcal{G}_{ij}}(\mathbf{c}) &= W_{ij}(\mathbf{c})\mathcal{G}_{ij}(\mathbf{c}) + W_{ji}(\mathbf{c})\mathcal{G}_{ji}(\mathbf{c}), \\ W_{ij}(\mathbf{c}),\ W_{ji}(\mathbf{c}) &\geq 0, \qquad W_{ij}(\mathbf{c}) + W_{ji}(\mathbf{c}) = 1, \end{aligned} \tag{9}$$

which is finally taken as the gradient estimate at the edge $\mathsf{e}_{ij}$.

The terms $W_{ij}(\mathbf{c})$ in equation (9) are the scalar weights of the final average and are generally assumed to depend on the set of neighbour cell-averaged and vertex-reconstructed values.

This approach generalises the *"diamond scheme" average* [3], which corresponds to a choice of the weights which depends only on the area of the closest cells,

$$W_{ij}(\mathbf{c}) = |\mathsf{T}_i| / (|\mathsf{T}_i| + |\mathsf{T}_j|),$$

but is independent from the cell-average solution values.

We propose a different and original *non-linear average*, where the weights are

$$W_{ij}(\mathbf{c}) = \begin{cases} \dfrac{|g_{ji}(\mathbf{c})|}{|g_{ij}(\mathbf{c})| + |g_{ji}(\mathbf{c})|}, & \text{if } |g_{ij}(\mathbf{c})| + |g_{ji}(\mathbf{c})| > 0 \\ 1/2 & \text{if } |g_{ij}(\mathbf{c})| + |g_{ji}(\mathbf{c})| = 0 \end{cases}$$

and $g_{ij}(\mathbf{c}) = \mathcal{G}_{ij}(\mathbf{c}) \cdot \mathbf{n}_{ij}$.

Finally, the integral of the numerical flux for the diffusive term in equation(3) is defined by

$$\mathrm{H}_{ij}(\mathbf{c}) = \widetilde{h_{ij}}(\mathbf{c})c_i - \widetilde{h_{ji}}(\mathbf{c})c_j, \tag{10}$$

where the factor $\widetilde{h_{ij}}(\mathbf{c})$ and its corresponding one without tilde, $h_{ij}(\mathbf{c})$, are such that

$$0 \leq h_{ij}(\mathbf{c}), \widetilde{h_{ij}}(\mathbf{c}) \leq 4d_{ij}\,\mathrm{cotg}(\theta_{min}/2),$$

$\widetilde{c_{ij}} = \widetilde{c}(\cdot, \mathbf{x}_{ij})$, $\mathbf{x}_{ij}$ being the midpoint of the edge $\mathsf{e}_{ij}$, and the following relations hold

$$\begin{aligned} d_{ij}\,|\mathsf{e}_{ij}|\,\widetilde{\mathcal{G}_{ij}}(\mathbf{c}) \cdot \mathbf{n}_{ij} &= h_{ij}(\mathbf{c})(\widetilde{c_{ij}} - c_i) \qquad \text{for all } \mathsf{e}_{ij} \in \mathcal{E}_h, \\ h_{ij}(\mathbf{c})(\widetilde{c_{ij}} - c_i) &= \widetilde{h_{ji}}(\mathbf{c})c_j - \widetilde{h_{ij}}(\mathbf{c})c_i \qquad \text{for all } \mathsf{e}_{ij} \in \mathcal{E}_h^I. \end{aligned}$$

### 3.4. Numerical Approximation of the Source Term

The volume production/consumption source term is numerically discretized in every cell $\mathsf{T}_i \in \mathcal{T}_h$ by the second-order quadrature formula

$$\begin{aligned} S_i(\mathbf{c}) &= |\mathsf{T}_i|\, B(\cdot, \mathbf{x}_i, c_i) - |\mathsf{T}_i|\, A(\cdot, \mathbf{x}_i, c_i)c_i, \\ &= \int_{\mathsf{T}_i} B(\cdot, \mathbf{x}, c(\cdot, \mathbf{x})) - A(\cdot, \mathbf{x}, c(\cdot, \mathbf{x}))c(\cdot, \mathbf{x})\, d\mathbf{x} + \mathcal{O}\left(h^3\right). \end{aligned}$$

# 4. Formal Properties of the FV Formulation

In this section we introduce a matrix-like formalism that allows us to reformulate the FV scheme (4) in a more compact form. Using a suitable definition of the matrix operators $\mathbf{G}$, $\widetilde{\mathbf{G}}(\mathbf{c})$, $\mathbf{H}(\mathbf{c})$, $\mathbf{F}$, $\widetilde{\mathbf{F}}(\mathbf{c})$ and the vectors $\mathbf{f}$, $\widetilde{\mathbf{f}}(\mathbf{c})$ – see [2] for the details – the integral of the upwind numerical flux in (8) and of the diffusive numerical flux in (10) can be written as

$$\begin{aligned} \Big[\mathbf{G}\mathbf{c} - \widetilde{\mathbf{G}}(\mathbf{c})\mathbf{c}\Big]_i &= \sum_{j \in \mathcal{T}_h(i) \cup \mathcal{T}'_h(i)} \mathrm{G}_{ij}(\mathbf{c}), \\ \Big[\mathbf{H}(\mathbf{c})\mathbf{c}\Big]_i &= \sum_{j \in \mathcal{T}_h(i) \cup \mathcal{T}'_h(i)} \mathrm{H}_{ij}(\mathbf{c}), \end{aligned} \tag{11}$$

while the integral of the numerical flux at boundary edges takes the more compact form

$$\Big[\mathbf{F}\mathbf{c} - \widetilde{\mathbf{F}}(\mathbf{c})\mathbf{c} - (\mathbf{f} - \widetilde{\mathbf{f}}(\mathbf{c}))\Big]_i = \sum_{j \in \mathcal{T}'_h(i)} \mathrm{F}_{ij}(\mathbf{c}). \tag{12}$$

The r.h.s. source also takes a matrix-like form as

$$\mathbf{S}(\mathbf{c}) = \mathbf{b}^S(\mathbf{c}) - \mathbf{A}(\mathbf{c})\mathbf{c}. \tag{13}$$

Using the previous compact definitions (11), (12), and (13), we obtain the following matricial form of the FV scheme (4)

$$\frac{d}{dt}(\mathbf{M}\mathbf{c}) + \mathbf{N}(\mathbf{c})\mathbf{c} = \widetilde{\mathbf{N}}(\mathbf{c})\mathbf{c} + \mathbf{b}(\mathbf{c}),$$

where $\mathbf{b}(\mathbf{c}) = \mathbf{f} - \widetilde{\mathbf{f}}(\mathbf{c}) + \mathbf{b}^S(\mathbf{c})$ takes into account the discretization of the boundary conditions, and we introduced the non-linear matrix operators $\mathbf{N}(\mathbf{c}) = \mathbf{F} + \mathbf{G} + \mathbf{H}(\mathbf{c}) + \mathbf{A}(\mathbf{c})$ and $\widetilde{\mathbf{N}}(\mathbf{c}) = \widetilde{\mathbf{F}}(\mathbf{c}) + \widetilde{\mathbf{G}}(\mathbf{c})$. Under the assumptions given in the previous section it is possible to show both $\mathbf{N}(\mathbf{c})$ and $\widetilde{\mathbf{N}}(\mathbf{c})$ possess strong properties, that we formalize in the next propositions. The proofs are in [1].

**Proposition 3 (Properties of the Matrix Operators)**

1. $\mathbf{N}(\mathbf{c})$ *is an M-matrix;*
2. $\widetilde{\mathbf{N}}(\mathbf{c})$ *is a Stieltjes matrix.*

Two discrete analogues of Propositions 1 and 2 also hold. These are stated by the following two propositions.

**Proposition 4 (Non-Negativity)**
*The analytical property 1 becomes:*

$$\begin{array}{llll} \textit{if} & c_i(0) \geq 0, & \textit{for all } \mathsf{T}_i \in \mathcal{T}_h; & \\ & \mathsf{g_d}_\alpha(t) \geq 0, & \textit{for all } \alpha \in \mathcal{V}'_h, & t > 0; \\ & \mathsf{g_n}_{ij}(t) \geq 0, & \textit{for all } \mathsf{e}_{ij} \in \mathcal{E}_h^N, & t > 0; \\ \textit{then} & 0 \leq c_i(t), & \textit{for all } \mathsf{T}_i \in \mathcal{T}_h & t > 0. \end{array}$$

**Proposition 5 (Global Maximum Principle)**
*The analytical property 2 becomes:*

$$
\begin{array}{lll}
\textit{if} & c_i(0) \geq 0, & \textit{for all } \mathsf{T}_i \in \mathcal{T}_h; \\
 & \mathsf{g}_{\mathsf{d}\alpha}(t) \geq 0, & \textit{for all } \alpha \in \mathcal{V}'_h, \quad t > 0; \\
 & \mathsf{g}_{\mathsf{n}ij}(t) = 0, & \textit{for all } \mathsf{e}_{ij} \in \mathcal{E}_h^N, \quad t > 0; \\
 & b^S(\mathbf{c}) = 0, & t > 0; \\
\textit{then} & 0 \leq c_i(t) \leq M(t), & \textit{for all } t > 0.
\end{array}
$$

## 5. Conclusions

A FV scheme is proposed to solve the time-dependent reaction-advection-diffusion for the contaminant transport in porous media. The scheme is based on a special limited reconstruction for gradients within cells and at mesh edges. The introduction of a suitable matrix-like formalism allows us to reformulate the scheme in a more compact way. The matrix operators that appear in the new formulation show strong properties (M-matrices, Stieltjes matrices). Finally we mention that using these properties it is possible to prove that under quite general assumptions the discrete solution is non-negative and there holds a global maximum principle.

## References


[1] E. Bertolazzi and G. Manzini. *A Finite Volume scheme for contaminant transport in porous media.* Technical report, IAN-CNR (2000).

[2] —. *Limiting strategies for polynomial reconstructions in Finite Volume approximations of the linear advection equation* (2002). In this proceeding.

[3] Y. Coudière, J.-P. Vila and P. Villedieu. *Convergence rate of a finite volume scheme for a two-dimensional convection-diffusion problem.* M2AN. Mathematical Modelling and Numerical Analysis, **33** (1999) 493–516.

[4] R. Eymard, T. Gallouët and R. Herbin. *Finite Volume methods.* In *Handbook of numerical analysis, Vol. VII* (North-Holland, Amsterdam, 2000), pages 713–1020.

[5] C. Gallo and G. Manzini. *A fully coupled numerical model for two-phase flow with contaminant transport and biodegradation kinetics.* Communications in Numerical Methods in Engineering, **17** (2001) 325–336.

[6] D. Gilbarg and N. S. Trudinger. *Elliptic partial differential equations of second order* (Springer-Verlag, Berlin, 2001). Reprint of the 1998 edition.

[7] P. Jawahar and H. Kamath. *A high-resolution procedure for Euler and Navier-Stokes computations on unstructured grids.* J. Comput. Phys., **164** (2000) 165–203.