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A non-linear finite volume method coupled with a higher order MUSCL-type formulation for the numerical simulation of groundwater solute transport

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Abstract. A groundwater solute transport model that predicts the process of contaminant migration plays an important role in the control and remediation of groundwater contamination. For example, in simulating solute transport in groundwater, reliable prediction of fluid dynamics requires a simulator capable of correctly handling highly heterogeneous and anisotropic permeability tensors on nonorthogonal grids due to the complex geology of the aquifer. To solve the equations that constitute the flow model, simplifying assumptions must be made about the aquifer and the physical processes that govern groundwater flow. In this study, we applied an improved numerical formulation that deals with highly heterogeneous and anisotropic media and can handle distorted grids. The governing equations are solved via an implicit pressure and explicit concentration procedure, where the advective term is solved using a Monotonic Upstream Centered Scheme for Conservation Laws (MUSCL) type method. This method is based on a gradient reconstruction obtained by a least square technique in which the monotonicity is enhanced by a multidimensional limiting process (MLP). The essence of the present limiting strategy is to control the distribution of both cell-centered and cell-vertex concentration in a multidimensional way to flow physics. Is showed in the literature that this strategy satisfies the local extremum diminishing condition in a truly multidimensional manner. The dispersion term is discretized by a nonlinear two-point flux approximation method (NL-TPFA). This method is very robust and able to exactly reproduce piecewise linear solutions through a linear-preserving interpolation with explicit weights. The methods can be used with general polygonal meshes, although we restrict ourselves to conformal triangular and quadrilateral grids. To validate the adopted formulations, some benchmark problems found in literature are solved. These numerical experiments indicate that our formulations can provide robust solutions for simulating groundwater solution processes, especially in aquifer systems with complex physical and geological properties.

Keywords: Groundwater solute transport, Finite volume method for groundwater simulation, Nonlinear TPFA, MUSCL with MLP.

1 Introduction

Groundwater is one of the most important resources in the world. This resource is fundamental for many areas, such as, for use industrial, domestic, and agricultural usage. An aquifer is a geological formation, consider as an ”open” system, in this sense, groundwater may exchange mass and energy with its neighboring systems (soil, air, and surface water) through adsorption, ion-exchange, infiltration, evaporation, inflow, outflow, and other exchange forms. Thus, the quantity and quality of groundwater may vary with environmental changes and human activities. Due to population growth, and industrial and agricultural development, more and more groundwater is extracted, especially in arid areas. If the groundwater management problem is not seriously considered, over-extraction may lead to groundwater mining, salt water intrusion, and land subsidence. In fact, the quality of groundwater is gradually deteriorating throughout the world, becoming a global problem threatening human health and destroying the ecological environment (Sun and Sun [1]). Developing computational robust and accurate groundwater solute transport models is essential for understanding the contaminant transport processes. To

date, various simulators for groundwater solute transport models have been developed to predict the contaminant transport process in groundwater, such as, FEFLOW (Trefry and Muffels [2]) and MODFLOW (Panday [3]).

The classical numerical methods that are used to solve the governing equation of the groundwater solute transport are based in the Finite Element Method (FEM) and the Finite Difference Method (FDM). The classical five-point (in 2-D) FDM is not flexible for complex geometries and/or unstructured grids, i.e., it may lose accuracy when predicting solute concentrations, on the other hand, the classical FEM does not conserve mass locally and is can not be applied to arbitrary polygon grids, although, the FEM has much more flexibility for representing complex geometries that FDM (Carvalho [4])

In this sense, in the present work we propose a full Finite Volume Method (FVM) to handle the flow and the transport problems, that is flexible to handle unstructured meshes and produces monotone solutions even problems with highly anisotropic porous media. In this study, a groundwater solute transport model on unstructured grids cells is established using a variant based on the FVM. This method satisfies the following properties: local conservation and monotonicity of approximate solutions, i.e., it preserves positive solutions whenever it is the case. Moreover, the scheme satisfy the linearity-preserving criterion and achieve second-order accurate for general polygonal meshes for smooth solutions, and in the presence of full coefficient tensors. For instance, in the context of petroleum reservoir simulation, the lack of monotonicity or DMP (Discrete Maximum Principle) of the numerical solutions may lead to the creation of spurious oscillations on the pressure field. For some problems of practical interest, such as oil reservoir, this is related to the appearance of spurious gas in regions of the reservoir, where the pressure falls erroneously below the bubble point (Contreras et al. [5]). Besides, these inaccurate pressure fields may induce non-physical Darcy velocities (Contreras et al. [6]). In this paper, the dispersive flux and the pressure field and Darcy flux are approximated using a variant of the non-linear FVM originally proposed by Yuan and Sheng [7] and Wu and Gao [8] to solve diffusion problems and used by Contreras et al. [5] in the oil reservoir simulation context. The non-linear Two-Point Flux Approximation (NL-TPFA) produces monotone solutions on any star-shaped polygonal meshes and arbitrary anisotropic diffusion tensors, these advantages are important in groundwater simulation. Moreover, our scheme uses a linearity-preserving interpolation with explicit weights originally proposed by Gao and Wu [9]. In order to accelerate the Picard iterations, we use the Anderson Acceleration method (Contreras et al. [5]). The concentration on the control surface is approximated using the high-order MUSCL-type scheme together with the multidimensional limiting process (MLP). This limitation strategy was initially proposed by Park et al. [10] for solving aerodynamics problems, afterwards Souza et al. [11] has used it in oil reservoir simulation context.

2 Governing equations

In this section, the governing equations for the groundwater contaminant problem, is describe briefly following the simplifying hypothesis, that the fluid and rock are both incompressible, that the flow is isothermal and we neglecting the capillary pressure, gravitational and viscosity term. We also assume that the aquifer is fully saturated by water. The Advection-Dispersion equation is able to model the spatial and temporal evolution of chemical or biological substances within a fluid, and can be represented through the field of concentration:

$$\phi\frac{\partial c}{\partial t} + \nabla\cdot(\vec{v}c) + \nabla(-\mathbf{D}\nabla c) = 0. \tag{1}$$

where the constants ϕ and c represent the porosity and concentration, respectively. The hydrodynamic dispersion tensor is denoted by $\mathbf{D}$ and the Darcy velocity is given by $\vec{v} = -\mathbf{K}\nabla p$, where the variable p and $\mathbf{K}$ denote pressure and permeability tensor, respectively. After some algebraic manipulation, we can write the elliptic pressure equation $\nabla\vec{v} = Q$ in which the total fluid injection or production specific rate is denoted by Q,

2.1 Initial and boundary conditions

The governing equation described by Eq. (1) is completely determined when an appropriate set of initial and boundary condition are adopted:

$$
\begin{aligned}
p(\vec{x},t) &= p_D, \quad \text{on} \quad \Gamma_D \times [0,t], && (2)\\
\vec{v}\cdot\vec{n} &= \bar{g_1}_N, \quad \text{on} \quad \Gamma_N \times [0,t], && (3)\\
c(\vec{x},t) &= c_D, \quad \text{on} \quad \Gamma_D \times [0,t], && (4)\\
-\mathbf{D}\nabla c\cdot\vec{n} &= \bar{g_2}_N, \quad \text{on} \quad \Gamma_N \times [0,t], && (5)\\
c(\vec{x},t) &= c_0(\vec{x}), \quad \text{on} \quad \Omega \quad \text{and} \quad t=0. && (6)
\end{aligned}
$$

where Γ_N and Γ_D, represent the Dirichlet and Neumann boundaries, respectively. The p_D, c_D are known the scalar functions defined on Γ_D, on the other hand, the $\bar{g_i}_N$ are pre-defined on Γ_N. The initial conditions is given by $c_0(\vec{x})$.

3 Numerical formulations

In this section, the coupled equation (1) with the Darcy velocity is solved using the implicit pressure and explicit concentration strategy. In this strategy, initially, the pressure equation is solved implicitly by NL-TPFA, and the concentration field is solved explicitly, at each time step, computed according to the Courant–Friedrichs–Lewy (CFL) condition to maintain stability and the process repeats until the end of the simulation.

Discretization of the governing equation using finite volume method

The governing equation, given in Eq. (1), can be expressed in the integral form on a control volume $\hat{L}$, and after using the divergence and mean value theorems and the Euler forward explicit in time discretization transient term, we have:

$$
c_{\hat{L}}^{n+1} = c_{\hat{L}}^{n} - \Delta t \frac{1}{\phi V_{\hat{L}}} \left(\sum_{IJ\in E_{\hat{L}}} (\vec{f}_{adv}\cdot\vec{N})_{IJ} + (\vec{f}_{disp}\cdot\vec{N})_{IJ} \right)^{n}. \tag{7}
$$

In Eq. (7), the concentration on any cell $\hat{L}$ in the level time n is denoted by $c_{\hat{L}}^{n}$ and $V_{\hat{L}}$ is area in 2D (volume in 3D). On the hand, the advective and dispersive terms are denoted by $\vec{f}_{adv} = c\vec{v}$ and $\vec{f}_{disp} = -D\nabla c$, respectively. The term IJ represent a generic edge (2D) of the computacional mesh.

Discretization of the dispersive term using the NL-TPFA method

The dispersive term is approximated by the following expression:

$$
\sum_{IJ\in E_{\hat{L}}} (\vec{f}_{disp}\cdot\vec{N})_{IJ} = w(c)_{\hat{L},IJ} c_{\hat{L}} - w(c)_{\hat{R},IJ} c_{\hat{R}}. \tag{8}
$$

The concentrations on the left and right side to edge IJ (2-D) are denoted by $c_{\hat{L}}$ and $c_{\hat{R}}$, respectively. The coefficients $w(c)_{\hat{L},IJ}$ and $w(c)_{\hat{R},IJ}$ depend on the interpolated nodal concentration and the physical-geometrical parameters, for more details, see Contreras et al. [5].

Discretization of the advective term using higher order method

The advective flux on the control surface, can be written as:

$$
\vec{f}_{adv}\cdot\vec{N}_{IJ} = c_{IJ}\vec{v}_{IJ}\cdot\vec{N}_{IJ}, \tag{9}
$$

where the flow rate $\vec{v}_{IJ}\cdot\vec{N}_{IJ}$ is approximated using a NL-TPFA scheme, given by:

$$\vec{v}_{IJ} \cdot \vec{N}_{IJ} = w(p)_{\hat{L},IJ} p_{\hat{L}} - w(p)_{\hat{R},IJ} p_{\hat{R}}. \tag{10}$$

Here $p_{\hat{L}}$ and $p_{\hat{R}}$ denote the pressures on the left and right side to edge IJ, respectively. The weights $w(p)_{\hat{i},IJ}$, $\hat{i} = \hat{L}, \hat{R}$ depend on physical-geometrical parameters on the pressure unknowns defined at the vertices of the mesh (Contreras et al. [5]). The concentration on the edge IJ is denoted by c_{IJ}, this parameter is approximated using an Upwind strategy, as given in the following expression: $c_{IJ} = c_{\hat{L},IJ}$, if $\vec{v}_{IJ} \cdot \vec{N}_{IJ} \geq 0$ and $c_{IJ} = c_{\hat{R},IJ}$ otherwise. The variables $c_{\hat{L},IJ}$ and $c_{\hat{R},IJ}$ are approximated using the expression given in eq. (11).

Higher-order MUSCL-type finite volume scheme

The construction of the concentration on the edge IJ is approximated by the following expression:

$$c_{\hat{i},IJ} = c_{\hat{i}} + \frac{\psi_{\hat{i}}}{4} \left[(1-k)\Delta c_{\hat{i}} + (1+k)(c_{\hat{R}} - c_{\hat{L}}) \right], \quad \textit{where} \quad \hat{i} = \hat{L}, \hat{R}, \tag{11}$$

in Eq. (11), the parameter k is used to control the degree of approximation and $\Delta c_{\hat{i}} = 2\overrightarrow{x_{\hat{L}} x_{\hat{R}}} \cdot \nabla c_{\hat{i}} - (c_{\hat{R}} - c_{\hat{L}})$, where $\hat{i} = \hat{L}, \hat{R}$. In this case, the $\nabla c_{\hat{i}}$ is approximated using a modified Least-Square reconstruction. On the other hand, in order to preserve monotonicity, we use the multidimensional limiter (MLP) as described in what follows.

Multidimensional limiting process (MLP)

To maintain the monotonicity of the variables c_{IJ} in higher-order approximations, we use the multidimensional limiting process (MLP) proposed by Park et al. [10] and used by Souza et al. [11] in the oil reservoir simulation context. First, for the each vertex j, we have:

$$c_{min} \leq \tilde{c}_j \leq c_{max} \quad \textit{and} \quad \tilde{c}_j = c_{\hat{i}} + \nabla c_{\hat{i}} \cdot \overrightarrow{x_{\hat{i}} x_j}, \tag{12}$$

here, c_{min} and c_{max} are the maximum and minimum values, respectively, among all immediate neighboring of cell $\hat{i}$, including, itself.

The calculation of a local extrema for an arbitrary vertex j is given, by:

$$r = \frac{\Delta}{\tilde{c}_j - c_{\hat{i}}}, \tag{13}$$

in Eq. (13), $\Delta = c_{max} - c_{\hat{i}}$, if $\tilde{c}_j - c_{\hat{i}} > 0$ or $\Delta = c_{min} - c_{\hat{i}}$, if $\tilde{c}_j - c_{\hat{i}} < 0$. According to Park et al. [10], the sign of $\tilde{c}_j - c_{\hat{i}}$ is the key to this choice. Now, we can define the MLP slope limiter for each vertex j as: $\psi_{j,\hat{i}} = \min(1, r)$, if $\tilde{c}_j - c_{\hat{i}} \neq 0$ or $\psi_{j,\hat{i}} = 1$, if $\tilde{c}_j - c_{\hat{i}} = 0$. Finally, we have:

$$\psi_{\hat{i}} = \min(\psi_{j,\hat{i}}), \quad \textit{for each vertex } j \textit{ of } \hat{i}. \tag{14}$$

The cell-based limiter, defined in eq. 14, ensure that no concentration extrema appear for any face IJ of the evaluated control volume $\hat{i}$ this gives the multidimensional character of the MLP limiter.

4 Numerical experiments

In this section, we compare the results obtained by the proposed method with that obtained using a Multipoint Flux-Approximation with Diamond stencil (MPFA-D) initially used to solve diffusion problems (Gao and Wu [9]) and applied by Souza et al. [11] to simulate water-oil displacement in petroleum reservoir. Moreover, in order to check for the accuracy and robustness of the higher order scheme, the advective term was also approximated by the first order upwind method and the results are compared. In all tests, the CFL and porosity values are 0.6 and $\phi = 1$, respectively.

4.1 Contaminants transport from an upstream strip source

This non-dimensional example is adapted from Yeh [12] and Rees et al. [13], and consists in a contaminant injected with a constant flow rate in an upstream strip source, as shown in 1. In this case, the governing equation (1), can be simplified as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial}(D_{xx}\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(D_{yy}\frac{\partial c}{\partial y}) - v\frac{\partial c}{\partial x} \quad \textit{where} \quad 0 \leq x \leq 10, \;\; 0 \leq y \leq 5. \tag{15}$$

In this problem, the mean velocity is $v = (1, 0)$, the simulation time considered is $t = 2$, the Peclet number is 0.05. The hydrodynamic dispersion tensor is defined, by: $\mathbf{D} = diag(4, 0.04)$ and the permeability tensors is defined, as $\mathbf{K} = diag(10, 0.01)$. The initial condition for the concentration field is $c_0 = 0$ and the boundary conditions are given in Table 1.

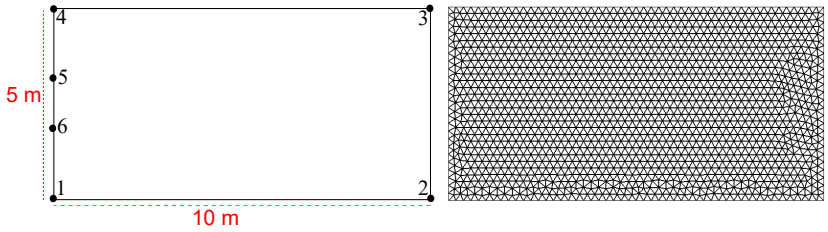

Figure 1. Contaminant transport from an upstream strip source: Physical domain (left) and triangular unstructured mesh ($\Delta x = 0.2$) with 2,932 cells (right).

Table 1. Contaminants transport from an upstream strip source: Boundary conditions for $t \geq 0$.

Boundary conditions	Pressure	Concentration
side 4-5 and 6-1	$p = 1$	$c = 0$
side 5-6	$p = 1$	$c = 1$
side 2-3	$p = 0$	$\frac{\partial c}{\partial x} = 0$
side 1-2 and 3-4	$\vec{v} \cdot \vec{n} = 0$	$\frac{\partial c}{\partial y} = 0$

In this problem, the increase of the dispersive coefficients ratio reduce the effect of the transverse dispersivity coefficient, the contaminant tends to concentrate along the x-axis so that the contamination "plume" becomes much narrower, reducing diffusion in the direction transverse to the flow.

In the top of Figure 2, the concentration field obtained by the MPFA-D/MUSCL-type with MLP scheme present negative values. This occurs due to the high anisotropy of the rock and due to the high ratio between the longitudinal and transversal components of the dispersion tensor. In counterpart, the concentration field obtained by NL-TPFA/MUSCL-type with MLP scheme is positive for all time steps (see Fig. 2 bottom).

4.2 Transport of tracer solutes from an upstream transient pulse

This problem was adapted from Lewis et al. [14] and Rees et al. [13]. In this case, we consider the computational domain of the problem 4.1 and an unstructured triangular mesh with $\Delta x = 0.5$, the injection contaminant acts for a given period of time $t = 1$ and the it stops. The hydrodynamic and permeability tensors are given by $\mathbf{D} = diag(0.004)$ and $\mathbf{K} = diag(10)$, respectively. The analytical solution was given by Van Genuchten [15]. This test is characterized to be strongly advective dominant because the Péclet number is 50.

Analyzing Fig. 3, we show that the greater accuracy of the high-order method is evident when compared with the First Order Upwind (FOU) method. We can notice that, the lower order scheme suffers from excessive artificial numerical diffusion, see Figs. 3 and 4 for more details.

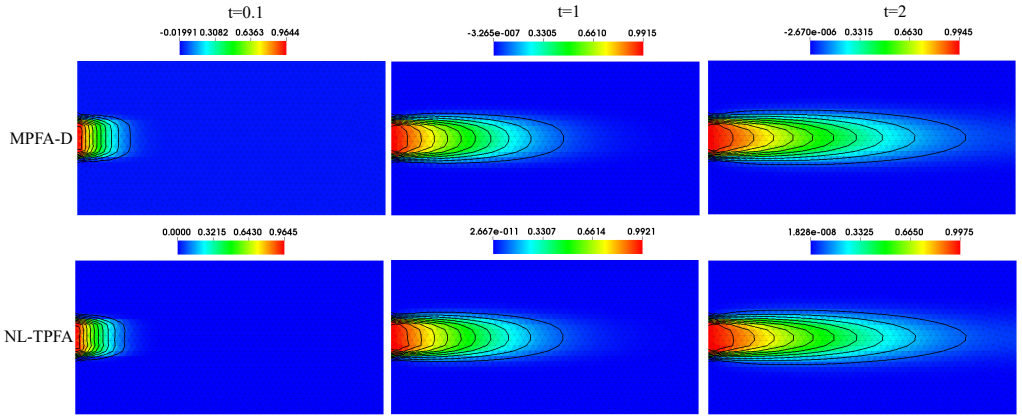

Figure 2. Contaminants transport from an upstream strip source: Concentration profile using MUSCL-type with MLP on triangle unstructured mesh with 2932 cells.

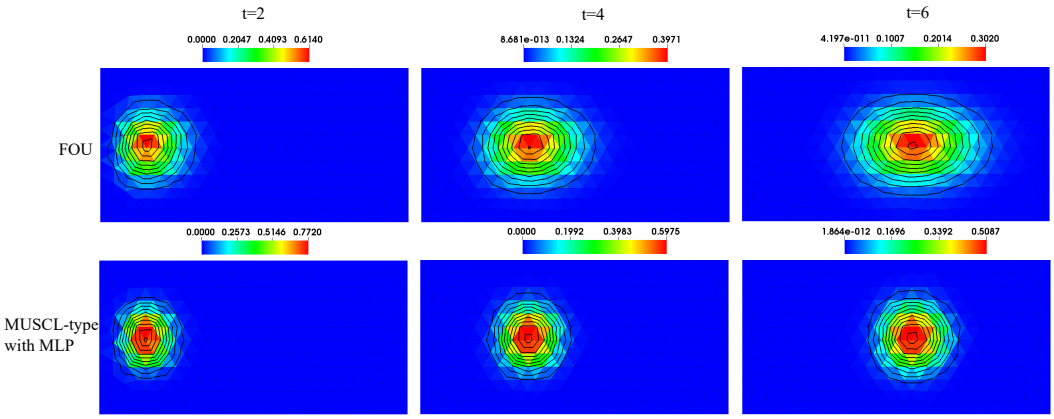

Figure 3. Transport of tracer solutes from an upstream transient pulse: Concentration profile using NL-TPFA/ FOU (top) and NL-TPFA/MUSCL-type with MLP (bottom) on the triangle unstructured mesh ($\Delta x = 0.5$) with 484 cells.

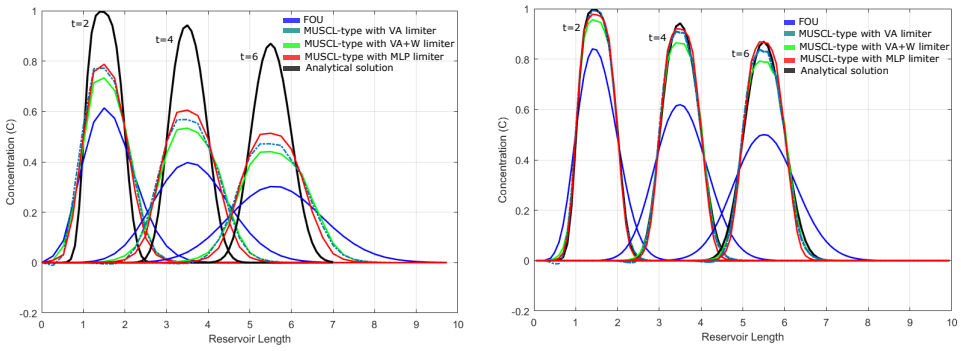

Figure 4. Transport of tracer solutes from an upstream transient pulse: Concentration distribution for different time stages obtained at $y = 2.5$ on triangular mesh with 484 cells (left) and with 2,932 cells (right).

5 Conclusions

In the present work, we propose a full finite volume formulation for the numerical approximation of the groundwater solute transport in non-homogeneous and non-isotropic porous media. To numerically approximate the dispersion term, we propose a monotone Non-Linear Two-Point Flux-Approximation (NL-TPFA) scheme that uses the Picard iteration procedure, whose efficiency is improved through the Anderson Acceleration method. To approximate the advective term, we use the MUSCL-type High-Order Finite Volume Method together with

multidimensional limiting process (MLP). Our results indicate that the proposed scheme considerably reduces artificial numerical diffusion significant improving the front resolution of the contaminant plume. As expected, in all cases, our formulation was able to produce positive concentration fields even for highly anisotropic dispersion tensors.

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