Introduction To High-Resolution Finite Volume Methods

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Hyperbolic partial differential equations (PDE), specifically *Conservation Laws* (these are PDEs usually used to represent some physical process where some variables are conserved) such as the one used to describe the advective-transport of pollutants, have long resisted accurate and cost-effective numerical solutions. Most numerical schemes are plagued by spurious oscillations or excessive numerical dispersion, both of which can be remedied only at the cost of very small time steps and grid spacing requiring large CPU time. One of the most successful schemes for the accurate solution of hyperbolic problems are those based on *High-Resolution Finite Volume methods* (HRFVM) and limiters constructed using the *Total Variation Diminishing* (TVD) principle. Our main goal is to review the basic concepts of HRFVM and TVD schemes and to introduce their use in the numerical solution of the transport of contaminants in porous media. However, the formalism is completely general and it can be used to solve any linear hyperbolic PDE. For non-linear PDEs the method is still useful, but some modifications must be introduced in order to handle the non-linear properties of the equation.

1 Introduction

We start the discussion looking at the PDE that we want to solve. The solute transport due to advection[1], i.e. due to the main movement of the water flow, in a three-dimensional domain is represented by:

$$\frac{\partial(\eta c)}{\partial t} = -\frac{\partial(u_i c)}{\partial x_i}, \quad \text{for} \quad i = 1, 2, 3 \tag{1}$$

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[1]In these notes we focus on the transport due to advection and we ommit the diffusion term. Note that the advection-diffusion equation is still a Conservation Law, but it is a parabolic PDE. The methodology described in these notes can be used to solve the advective term of the advection-diffusion equation if a *Splitting or Fractional Step method* is used to decouple the advective and dispersive terms (see Calhoun and Leveque (2000); Cirpka et al. (1999) for some examples of this approach).

where u_i is the pore water velocity in the i direction, x_i is one of the Cartesian component of the position vector $\mathbf{x} = (x, y, z)$, η is the porosity, and t is the time[2]. Mathematically, this PDE is part of a broader family called *Hyperbolic Conservation Laws* (HCL). For the sake of completeness we include a brief definition of the mathematical classification of HCL.

Hyperbolic Conservation Law

A PDE of the form (2):

$$\frac{\partial q}{\partial t} + A\frac{\partial q}{\partial x} = 0 \qquad (2)$$

where $q = q(t, x)$ (variable) and $A = A(x)$ (coefficient) can be scalar, vector or matrix. Equation (2) is said to be *hyperbolic* if all eigenvalues of A are real.

A conservation law in one-dimension has the form:

$$\frac{\partial q}{\partial t} + \frac{\partial f(q(x,t))}{\partial x} = \frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial q}\frac{\partial q(x,t)}{\partial x} = 0 \qquad (3)$$

where $f(q)$ is called the *flux function*. According to the previous definion (3) will be a *Hyperbolic Conservation Law* if the Jacobian of the flux function, i.e. $\frac{\partial f}{\partial q}$, has real eigenvalues (LeVeque, 2002).

In the case of the advection equation (1), we can identify $q = c$ and $f(q) = uc$. Other forms of HCL are used to described different physical phenomena such as: elastic waves, traffic flow, Navier-Stokes equation, neutron transport, and others. All of these phenomena share some common characteristics (Haber, 2003):

1. Information on the inflow boundary is propagated along the characteristics curves.

2. If data is discontinous at X_0 on the inflow boundary, then the solution will be discontinous everywhere along the characteristic curve passing through X_0.

3. The inflow boundary data fully determine the solution on the outflow boundary[3]. Therefore, we cannot prescribe c (or q in the general case) on both, the inflow and outflow boundaries.

What does that mean in the case of contaminant transport?

Let consider the following example: A storage tank is leaking a pollutant into an aquifer. In order to simulate this problem we make some simplifying assumptions: i) the tank can be consider a constant source of contaminant, ii) the flow of water in the aquifer is oriented in just one direction (i.e. flow is one-dimensional), iii) the flow is homogeneous (this would not be a good assumption for a real case where the velocity is highly variable in space), and iv) the effect

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[2]A detailed discussion of the derivation of (1) is covered in the section Topic III.A-C of the Class Notes.

[3]Actually, the solution is determined by the inflow and the source/sink term in the case of a non-homogeneous PDE.

of the hydodynamic dispersion is negligible. A cartoon of this situation is presented in Figure (1). In this situation the contaminant will move carried by the flow and the plume will advance as a *sharp front*.
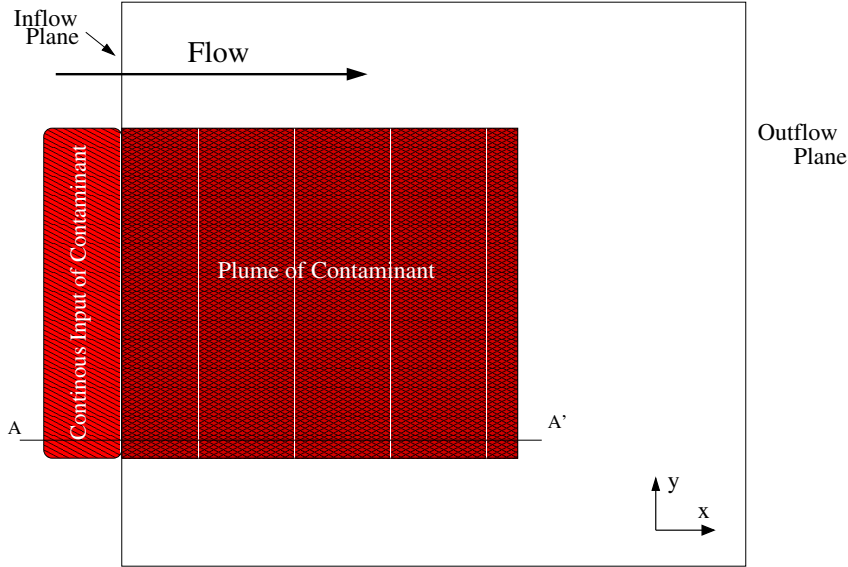

Figure 1: Transport of contaminant due to advection in a idealized aquifer.

Figure (2) shows the concentration profile along the AA' plane as a function of time. Here, we have made an extra assumption: the spilling started instantaneously and the concentration released is constant and equal to one. There are some important characteristics of the real solution of the problem shown in Figure (2) that we must consider when we chose a numerical method to find an approximate solution[4]: i) the solution of the problem described in (1) $c(x, t)$ is discontinous at location x^* at time t^*, and ii) the discontinuity or front advances in time following the characteristic curve. Moreover, the derivative of $c(x, t)$ respect to x is not defined at $x = x^*$.

The fact that the solution is discontinuous is the major obstacle to finding an accurate numerical solution for (1). Traditional numerical techniques such as Finite Difference (FD)and Finite Elements (FEM) consider that the solution is continuous at every point. In fact, FD methods approximate the first derivative of the flux that appears in (1) as a discrete expression, assuming that it does exist in all the domain. On the other hand, FEM expresses the solution as a sum of continuous polynomial basis functions.

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[4]Of course we will use numerical methods in more complicated situations where it is not easy or it is imposible to find an analytical solution of (1). For example, situations with non-uniform velocity fields or strange geometries. However, the solution of those problems still have these same features.
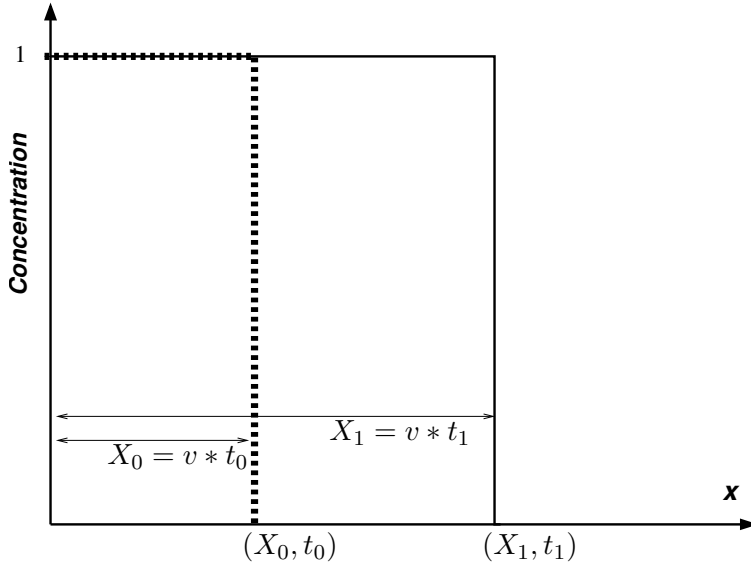
Figure 2: Concentration profile as a function of distance x.

More recent numerical techniques such as Finite Volume (FVM) (LeVeque, 2002; Toro, 1997; Chilakapati et al., 2000; Farthing and Miller, 2001; Cirpka et al., 1999) and Discontinous Galerkin Finite Elements (DGFEM) (Cockburn et al., 2000, 1990; Cockburn and Shu, 1998a, b; Dawson et al., 2000; Riviere et al., 2000; Riviere and Wheeler, 2000) methods do not assume *a priori* continuous solution. The FVM works based on an integral form of (1) and they do not compute the derivative of the flux function but rather some approximation to the fluxes. On the other hand, DGFEM utilize *discontinuous basis function*, relaxing the interelement continuity condition of standard FEM. The next sections present some of the mathematical formalism of FVM and their implementation to solve (1).

2 Mathematical Formalism

In the following discussion we will consider the one-dimensional case because it is easier to understand. Furthermore, the numerical solution of many multidimensional problems can be easily computed through the succesive aplication of one-dimensional methods as explained later. We will particularly focus on FVM based on the Godunov's appoach to solve Hyperbolic Conservation Laws. Those methods solve the hyperbolic equation based on an integral form. Thus, it can solve problems with discontinuous solutions and it overcomes most of the difficulties of traditional Finite Difference techniques for those cases. The basic idea is to "... break the domain into grid cells and approximate the total integral of c over each grid cell, or actually the *cell average* of c ..." (LeVeque, 2002). Figure (3) shows a schematic of the fluxes and average concentrations over a cell. To use FVM it is necessary to re-write (1) in terms of the fluxes and temporal mass variation to get (4) (Note: we drop the porosity η on the left side to simplify the notation). Equation (4) is the *integral form* of mass balance over the control volume Δx. The solution of (4) is called the *weak* solution of (1), because it does not require differentiability

(LeVeque, 1992)[5].

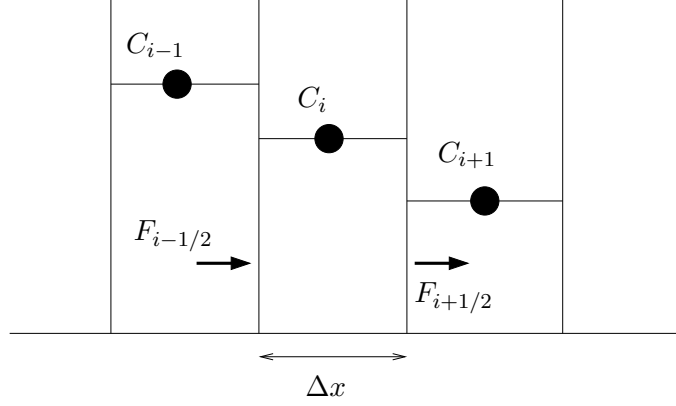$$\frac{d}{dt} \int_{\Delta x} c(x,t)dx = f(c(x_1,t)) - f(c(x_2,t)) \qquad (4)$$

Figure 3: Fluxes that affect the mass balance of cell i.

After integrating (4) in time from to t_n to t_{n+1}, dividing by Δx, and replacing c and f by discrete values, we obtain a discretized equation (5), where n and $F_{i\pm1/2}$ is an approximation to the temporal integral of the flux at the edge $i \pm 1/2$ in the interval of time Δt, as shown in (6).

$$C_i^{n+1} = C_i^n + \frac{\Delta t}{\Delta x}(F_{i-1/2}^n - F_{i+1/2}^n) \qquad (5)$$

$$F_{i-1/2}^n = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(c(x_{i-1/2},t))dt \qquad (6)$$

2.1 Godunov Method

From another point of view, the solution of (5) can be seen as the simultaneous solution of two Riemann problems at the left and right edge of the cell (Toro, 1997; LeVeque, 2002). Therefore, there are two approaches that are commonly used to solve (5). The first is based on the solution of the Riemann problem by using the *Reconstruct-Evolve-Average* (REA) algorithm proposed by Godunov (1959) that is used to define the average fluxes F.

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[5]The formal discussion of weak and true solution of (1) is beyond the scope of these notes. However, it is convenient to notice that the weak solution requires less smoothness (or differentiability), but it must be *integrable* according to some definition of integration(LeVeque, 1992; Haber, 2003). In particular, a discontinuous function can be integrabable *but not* differentiable. For practical purposes we can say that both solutions are similar in smooth regions where the function is continuous and differentiable, but they can be different near discontinuities.
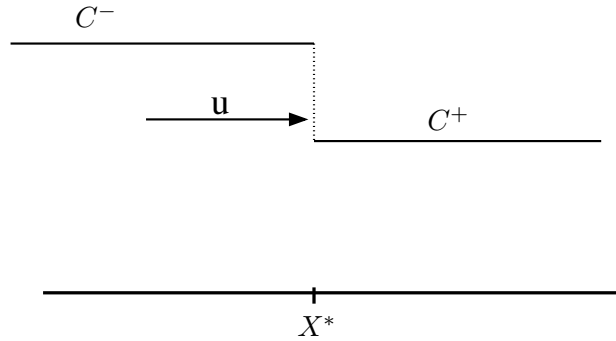
Riemann Problem

Mathematically the Riemann problem is defined by a hyperbolic PDE and a discontinuous initial condition:

$PDE:$ $\qquad \frac{\partial c}{\partial t} + \frac{\partial(uc)}{\partial x} = 0$

$IC:$ $\qquad c(x,0) = c_0(x) = \begin{cases} c^- & if \quad x < x^* \\ c^+ & if \quad x > x^* \end{cases}$

Graphically,

PSfrag replacements

Note by solving (5) we want to find the new mass distribution at time level $n+1$. That is, given the initial mass distribution at time level n (C^n) we want to know how much mass was transfered from the upstream cell. To compute the new mass we can solve the Riemann problem, i.e. to compute the displacement of the front and then re-distribute the new mass over each cell (calculating a new average C_i). Figure (4) shows a diagram of this procedure.

The re-distribution of mass in each cell can be achieved by using the REA algorithm that involves:

Algorithm 1 The Reconstruct-Evolve-Average (**REA**) algorithm.

1. Reconstruct a polynomial function $c_i(x, t_n)$ based on the cell average C_i,

2. Evolve the hyperbolic equation with this initial data (shift the inital data acoording to the solution of the Riemann problem),

3. Average the new function over each grid cell to get a new value of C_i at time t_{n+1}.

If a polynomial of degree zero is used to represent the concentration within each cell, i.e. a constant distribution as shown in Figure (3), this approach is numerically identical to the traditional *Upwind* applied in Finite Difference (FD) (Toro, 1997). In that case, the new average concentration can expressed as
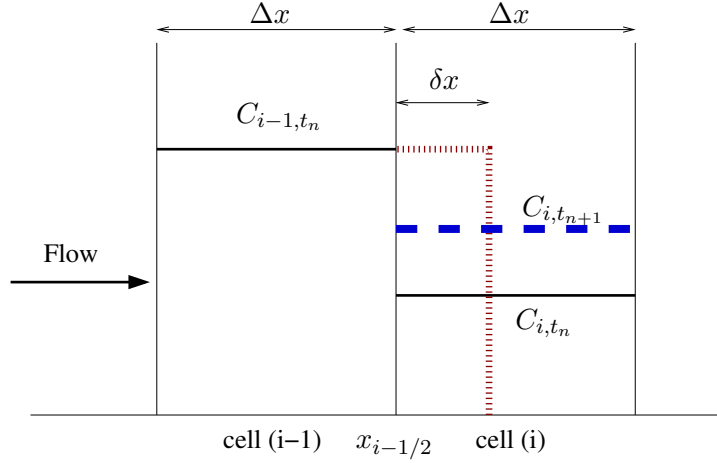
Figure 4: Redistibution of mass and Riemann problem. Initially the concentration in the cells i and (i-1) are constant. There is a discontinuity at x(i-1/2). At the new time level the concentration in cell i will be $C(i, t_{n+1}) = \frac{C(i-1,t_n)*dx + C(i,t_n)*(Dx-dx)}{Dx}$

$$C_i^{n+1} = C_i^n + \frac{v\Delta t}{\Delta x}(-\Delta C_{i-1/2}) \tag{7}$$

where $\Delta C_{i-1/2} = C_i - C_{i-1}$ is the jump of $C(x,t)$ at $x = x_{i-1/2}$.

There is a second approach that is based on the idea that is possible to express (7) in a discrete flux-differencing form (5). Therefore, the solution of the Riemann problems or the correct approximation of the fluxes are equivalent. For the specific case of the advective transport the approach based on the computation of the fluxes seems logical and straigthforward. However, for non-conservative hyperbolic problems the solution cannot be expressed as a discrete flux form (5) and the approach based on the true or approximated solution of the Riemann problem must be used (Toro, 1997). Some authors (Toro, 1997; LeVeque, 2002) expressed the fluxes in term of the solution of the Riemman problem, the jump and its velocity of propagation. In that case, they first solve the Riemann problem and then they compute the equivalent fluxes to substitute in the flux-differencing expression (5). It is straightforward to show that by substituting the average temporal integral of the fluxes as equal to the product of the immediate upstream concentration and velocity,

$$
\begin{aligned}
F_{i+1/2} &= v_{i+1/2}C_{i+1/2} = v_{i+1/2}C_i \\
F_{i-1/2} &= v_{i-1/2}C_{i-1/2} = v_{i-1/2}C_{i-1}
\end{aligned} \tag{8}
$$

in (5) we solve the left and right Riemann problem and we obtain the same expression (7) to compute a new concentration distribution C_i.
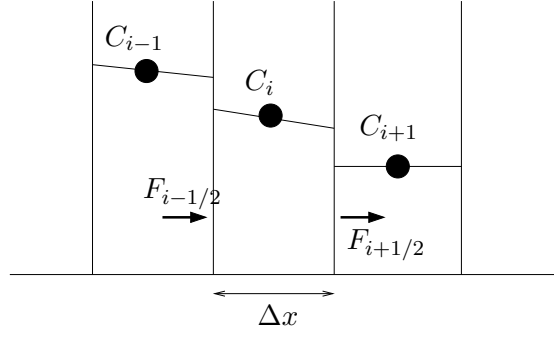
Figure 5: High-resolution first-order polynomial reconstruction of the concentration distribution within each cell.

2.2 High-resolution methods

A popular idea to improve the order of accuracy of the first-order Godunov's method is to consider a polynomial of higher degree to represent the mass distribution within each cell as shown in Figure (5). This idea is similar to the one applied in the Discontinuous Galerkin Finite Element (DGFEM). As in the case of DGFEM the order of accuracy of the solution depends upon the polynomial order used to represent $c(x,t)$ in step i) of the REA algorithm. High-order FVM are based on at least a first-order polynomial representation of $c(x,t)$.

When higher-order methods are used the modification of the distribution of concentration at each interface of the original Riemann problem produces the so called *Generalised Riemann Problem* (GRP) defined by (Toro, 1997). For the case of first-order reconstruction (second-order method) the GRP is:

$$PDE: \qquad \frac{\partial c}{\partial t} + \frac{\partial (vc)}{\partial x} = 0$$

$$IC: \qquad c(x,0) = c_0(x) = \left\{ \begin{array}{ll} c_{i-1}(x) & \text{if} \quad x < x_{i-1/2} \\ c_i(x) & \text{if} \quad x > x_{i-1/2} \end{array} \right. \tag{9}$$

In this case the new concentration given by the REA algorithm is

$$C_i^{n+1} = C_i^n - \frac{v\Delta t}{\Delta x}(C_i^n - C_{i-1}^n) - \frac{1}{2}\frac{v\Delta t}{\Delta x}(\Delta x - u\Delta t)(m_i^n - m_{i-1}^n) \tag{10}$$

where m_i is the slope of the reconstruction concentration $c(x)$ in cell i at time t_n. For the GRP the flux formulation requires that we compute the average time integral of the fluxes as

$$F^n_{i-1/2} = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} vc(x_{i-1/2}, t)dt$$

$$= \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} v(C^n_{i-1} + (x_{i-1/2} - v(t - t_n) - x_{i-1})m^n_{i-1})dt$$

$$= vC^n_{i-1} + \frac{1}{2}v(\Delta x - v\Delta t)m^n_{i-1} \tag{11}$$

So, if we compute the fluxes as in (11), and substitute into the flux-differencing form (5), we get the same same results as (10).

2.3 TVD Flux Limiters

As in the case of Runge-Kutta DGFEM (RKDG FEM), some limiters must be applied to avoid spurious oscillations near discontinuitites that are characteristic in high-order approximation. If we consider the piecewise polynomial reconstruction of $c(x,t)$ and the solution obtained using the REA algorithm (10) we talk about *slope limiters*, whereas if we use the discretized equation (11) we utilize the term *flux limiters*. Both approaches are equivalent and we can define a flux limiter for every slope limiter. Farthing and Miller (2001) and LeVeque (2002) present a complete survey of different slope/flux limiters.
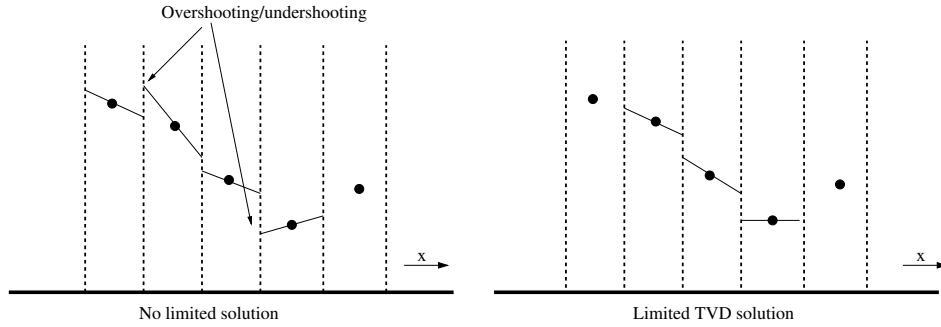

Figure 6: The non-limited version of the reconstruction introduces some overshooting/undershooting near discontinuities. The TVD version controls the reconstruction avoiding oscillations but decreasing the accuracy of the method near discontinuity (reproduced from LeVeque (2002)).

The notion of *total variation* of a function is usually used to construct flux limiters that guarantee monotonic solutions free of spurious oscillations.

Total Variation Dimishing (TVD)

The total variation of a discrete set of cells is defined as:

$$TV(C) = \sum_{i=1}^{n} \mid C_i - C_{i-1} \mid \qquad (12)$$

A method is said to be Total Variation Dimishing (TVD) if it produces solutions that satisfy (13). It has been proved that any TVD method preserves the monotinicity of a monotic solution.

$$TV(C^{n+1}) < TV(C^n) \qquad (13)$$

The basic idea of use of limiters is expressing the fluxes as:

$$F_{i-1/2}^n = F_L(C_{i-1}, C_i) - \Phi_{i-1/2}^n [F_H(C_{i-1}, C_i) - F_L(C_{i-1}, C_i)] \qquad (14)$$

F_L is the low-order flux and F_H is the high-order approximation of the flux. The function Φ is the flux limiter. When $\Phi = 0$ we obtain the low order method, and when $\Phi = 1$ eqn. (14) represents a high-order method. Methods that use limiters to control oscillations change the value of the limiter Φ to switch between high-order approximations in smooth regions to low-order methods near discontinuities.

The construction of TVD flux limiters is based on the following theorem:

Theorem

(This theorem was originally proposed by Harten. We used LeVeque (2002) as reference)

Consider a general method of the form:

$$C_i^{n+1} = C_i^n - \alpha_{i-1}^n (C_i^n - C_{i-1}^n) + \beta_i^n (C_{i+1}^n - C_i^n) \qquad (15)$$

over one time step, where the coefficients α_{i-1}^n and β_i^n are arbitrary values (which may depend on values of C_k^n). Then, the method will be TVD (i.e., it will satisfy (13)) if:

$$\alpha_{i-1}^n \geq 0 \quad \forall i$$
$$\beta_i^n \geq 0 \quad \forall i$$
$$\alpha_i^n + \beta_i^n \leq 1 \quad \forall i \qquad (16)$$

To get a general TVD method we must use a limited version of F in (11). We construct the

flux F for positive or negative velocities at the edge ($v_{i-1/2} > 0$ or $v_{i-1/2} < 0$) as

$$F^n_{i-1/2} = v^- C^n_i + v^+ C^n_{i-1} + \frac{1}{2} \mid v \mid (1 - \mid \lambda \mid) \delta^n_{i-1/2} \tag{17}$$

where $\lambda = \frac{v \Delta t}{\Delta x}$ is the CFL number, $v^- = min(0, v)$ and $v^+ = max(0, v)$, and

$$\delta^n_{i-1/2} = \phi(\theta^n_{i-1/2}) \Delta C^n_{i-1/2} \tag{18}$$

is a limited version of the jump, and

$$\theta^n_{i-1/2} = \frac{\Delta C^n_{I-1/2}}{\Delta C^n_{i-1/2}} \quad I = i - 1 \quad \text{if} \quad v > 0 \quad \text{or} \quad I = i + 1 \quad \text{if} \quad v < 0 \tag{19}$$

The function ϕ is defined as a *flux limiter*. There are several expressions to define it depending on the method and order of accuracy that we want to use.

Considering that $u > 0$, substituting (17) into (5), and applying a first-order explicit approximation in time we obtain a new expression for the new concentration (LeVeque, 2002):

$$C^{n+1}_i = C^n_i - \lambda(C^n_i - C^n_{i-1}) - \frac{1}{2}\lambda(1 - \lambda)[\phi(\theta^n_{i+1/2})(C^n_{i+1} - C^n_i)$$
$$- \phi(\theta^n_{i-1/2})(C^n_i - C^n_{i-1})] \tag{20}$$

Note that it is possible to use the previous theorem (16) to find the conditions that must be satisfied by (20) in order to get a TVD method. In particular , we can recast (20) in the form (15) identifying:

$$\alpha^n_{i-1} = \lambda + \frac{1}{2}\lambda(1 - \lambda)\frac{\phi(\theta^n_{i+1/2})}{\theta^n_{i+1/2}} - \phi(\theta^n_{i-1/2}) \tag{21}$$

$$\beta^n_i = 0$$

where we have used

$$C^n_{i+1} - C^n_i = \frac{C^n_i - C^n_{i-1}}{\theta^n_{i+1/2}} \tag{22}$$

The TVD conditions (16) are satisfied if:

1. $0 \leq \alpha^n_{i-1} \leq 1$, that is true if the CFL condition $0 \leq \lambda \leq 1$ holds, and

2. $0 \leq \phi(\theta) \leq minmod(2, 2\theta)$, where the *minmod* function is defined by:

$$minmod(a_1, a_2, \ldots, a_n) = \begin{cases} s \cdot min \mid a_i \mid & \text{if} \quad s = sign(a_1) = \ldots = sign(a_n) \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

Table 1 shows a summary of the most common flux limiters (Farthing and Miller, 2001; LeVeque, 2002). The *minmod* flux limiter corresponds to the lower bound of the TVD region defined

11

Limiter	$\phi(\theta)$
Upwind	0
Central	1
Superbee	max[0,min(1,2θ),min(2,θ)]
Minmod	minmod(1,θ)
MUSCL	max[0,min(1+θ/2,2,2θ)]
van Leer	$\frac{\theta+|\theta|}{1+|\theta|}$
ULTIMATE	max[0, min(2, 2 θ, $\frac{2-\lambda+\theta(1+\lambda)}{3}$]

Table 1: TVD flux Limiters.

in the plane (ϕ, θ) and gives solutions that are smooth and affected by some numerical dispersion. The Superbee flux limiter defines the upper bound of the TVD region and produces solutions that are sharp and well defined, but it is not suitable for some problems where it can introduce too much compression of the solution. The MUSCL and van Leer limiters are considered an intermediate alternative between minmod and Superbee limiters, therefore they are advised as a good choice for most problems.

Figure 7 shows a comparsion of the solutions given by different limiters for a problem of advection of an initial pulse. We used CFL=0.8 and we show the solution after 50 time steps. We observe the behavior of the solution agrees with the description of the limiters given above. The analytical solution of this problem coresponds to the initial pulse displaced a distance $\Delta x = v\Delta t$ in the downstream direction. The solution given by the minmod limiter is more diffusive than the MUSCL, and this is more diffusive than Superbee.
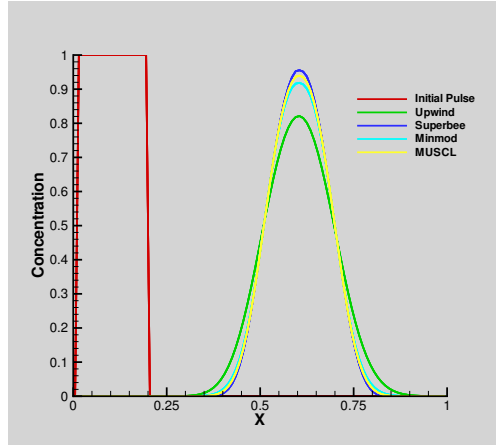

Figure 7: Comparison of the solution given by different flux limiters for the advective transport of an initial pulse.

2.4 Semi-discrete Approach

The exact solution of the GRP (9) problem is seldom used in practice. Instead, some approximation of the temporal integral of the fluxes is used in (5). The *semi-discrete* approach separates the temporal and spatial processes, transforming the PDE (1) into an Ordinary Differential Equation (ODE) (24).

$$\frac{dC_i}{dt} = \frac{1}{\Delta x} \left[F_{i+1/2}(t) - F_{i-1/2}(t) \right] \tag{24}$$

The fluxes $F_{i\pm1/2}(t)$ at time t can be computed using Godunov's idea, i.e. they are calculated as the product of the immediate upstream concentration $c_{i-1/2}(t)$ times the velocity. The concentration can be computed as the *limited* reconstructed value at each time. For instance, for a linear reconstruction: $c_{i-1/2}(x_L, t) = C_{i-1}(t) + \frac{1}{2}m_{i-1}^L(t)$, where m_i^L is the limited slope of the reconstruction in cell i. The solution of the ODE can be achieved by using a first-order explicit or implicit Euler discretization or some higher-order Runge-Kutta scheme that guarantees the TVD condition (Shu, 1988; Thai et al., 1997). We have implemented this semi-discrete approach in our FVM code using a second-order Runge-Kutta method defined by

$$C_i^* = C_i^n + \Delta t \mathcal{L}(C^n)$$
$$C_i^{**} = C_i^* + \Delta t \mathcal{L}(C^*)$$
$$C_i^{n+1} = \frac{1}{2} \left(C_i^n + C_i^{**} \right) \tag{25}$$

where $\mathcal{L}(C^n)$ is a discretization of the right-hand side of (24) for which the forward Euler method,

$$C_i^{n+1} = C_i^n + \Delta t \mathcal{L}(C^n) \tag{26}$$

is a TVD method (LeVeque, 2002).

2.5 Extension to Multidimensional Domains

To implement a high-resolution FVM for two-dimensions we use a *directional-splitting* method (Strang, 1968; LeVeque, 1982; Toro, 1997; LeVeque, 2002). We simply apply a high-resolution TVD method in each direction. Figure 8 shows a schematic of this approach in a two-dimensional problem. We compute the solution in two steps, first we advect the plume in the x-direction and then we displace the solution in the y-direction. The error that this split introduces can be minimized by using a Strang splitting-operator. Thus, we compute the solution at the time level $n+1$ as

$$C^* = \Lambda_x \left(\frac{\Delta t}{2} \right) (C^n)$$
$$C^{**} = \Lambda_y \left(\Delta t \right) (C^*) \tag{27}$$
$$C^{n+1} = \Lambda_x \left(\frac{\Delta t}{2} \right) (C^{**})$$
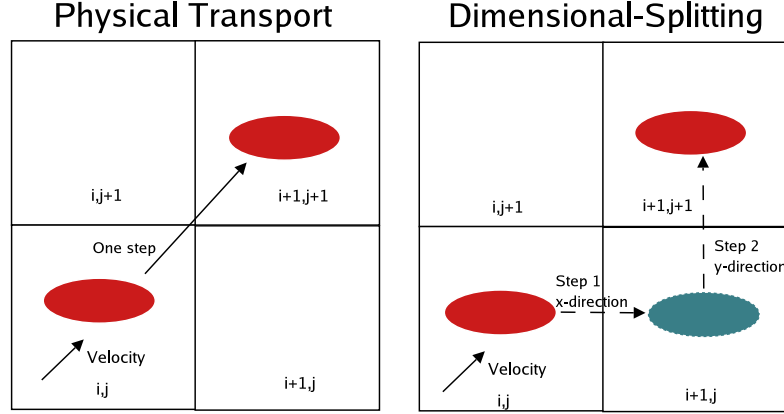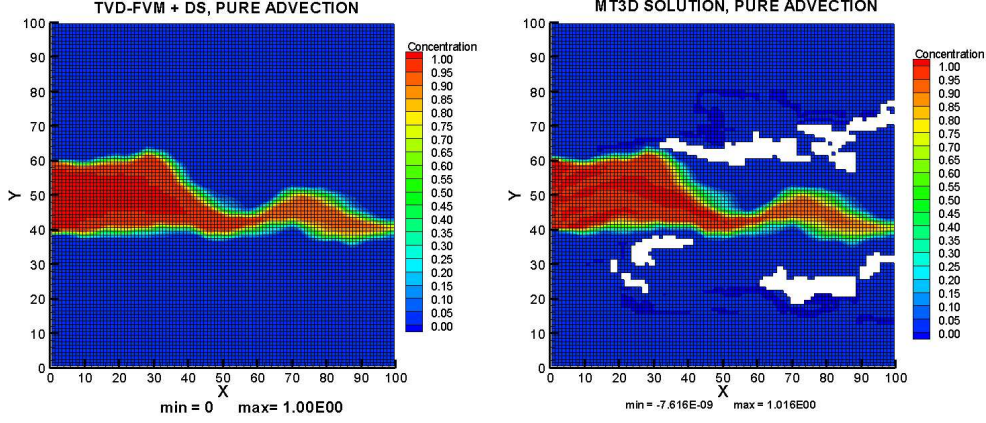
Figure 8: Dimensional-splitting approach.

where $\Lambda_j(\Delta)$ is the high-resolution operator in the direction j, applied during a time step Δ. There are some theoretical proofs that if Λ is a monotone operator for the one-dimensional conservation law, the solution given by the dimensional-splitting converges to the weak solution of the two-dimensional scalar conservation law as discussed by LeVeque (2002). The directional splitting approach gives a method that has the same stability restriction of a one-dimensional high-order FVM. This limit is

$$max \mid \frac{v_i \Delta t}{\Delta x} \mid \le 1 \quad i = x, y \tag{28}$$

There are other multidimensional methods known as *Unsplit* methods in which the fluxes in all the directions are computed at the same time step. In order to control oscillations, one-dimensional TVD flux limiters are applied in each direction, these schemes "...are usually referred to, *incorrectly, as two-dimensional TVD schemes*..." (Toro, 1997, page 529). One of those methods has been implemented in the popular MT3D solute-transport package (Zheng and Wang, 1999). There are four main advantages of the Directional-Splitting approach that we have implemented over *Unsplit* methods (Toro, 1997; LeVeque, 2002): i) any one-dimensional method can be extended to multidimensions, ii) the stability limits in the multidimensional and one-dimensional case are the same, iii) the implementation of Directional-Splitting is straightforward, and iv) the use of an unsplit method and one-dimensional TVD flux-limiters *does not* guarantee a TVD solution, i.e. there is no theoretical proof that the solution will be free of spurious oscillations. Figure 9 shows an example of the solution of advective transport in a heterogeneous hydraulic conductivity field given by the TVD-ULTIMATE solver included in MT3D and the directional splitting (DS) approach implemented in our 2D FVM code presented by Herrera and Valocchi (2003). We observe that the unsplit approach used in MT3D does not avoid spurious oscillations and negative concentration whereas the DS approach produces a monotonic positive solution.

The implemented FVM code includes first-order (upwind) and second-order (linear reconstruction) discretization in space. We have also implemented an explicit Runge-Kutta time dis-

(a) 2D FVM solution using Directional-Splitting and one-dimensional high-resolution TVD method.

(b) MT3D solution using the unsplit TVD UL-TIMATE solver, white regions represent negative concentrations.

Figure 9: Solution of two-dimensional advective transport in heterogeneous hydraulic conductivity field.

cretization in time that is second order $O(\Delta t^2)$. The Strang directional splitting also gives an error that is second-order in time $O(\Delta t^2)$. Thus, the complete method is formally second order in space and time for homogeneous velocity fields. However, in the case of a non-uniform velocity field ($v = v(x)$) the one-dimensional high-resolution method, even for the case when no flux-limiter is applied, is formally first-order accurate in space as discussed by LeVeque (2002), since the local truncation error is

$$error = -\frac{1}{2}[\Delta x - v(x)\Delta t]v'(x)\frac{\partial c(x,t)}{\partial x} + O(\Delta x^2) \qquad (29)$$

It is interesting to notice that the truncation error depends upon the spatial variation of the velocity field, i.e. upon the heterogeneity of the medium. A rapid spatial variation of the velocity introduces more error than a smooth variation. We have observed this behavior in our numerical simulations of advective transport in different random heterogeneous hydraulic conductivity fields.

3 Examples

We implemented the TVD formulation explained above in a FORTRAN90 code. To show the differences between HRFVM and traditional Upwind method, we simulated a 1D uniform velocity field, a 2D uniform velocity field, and a 2D non-uniform velocity field.

3.1 One-dimensional

We simulated a very simple 1D problem. We considered an initial "pulse" (plume) of solute of concentration C=1, in an uniform velocity field (u=constant). The parameters of this simulation are listed in Table (2).

Parameter	Value
Grid Spacing	0.05
Velocity	1.0
Time step Δt	0.025
CFL number	0.5

Table 2: Simulation parameters, 1D uniform velocity field.

The initial concentration and the results are shown in Figure (10). We observe that the TVD Superbee scheme captures and keeps the shape of the initial pulse. As expected the Upwind scheme has a significant amount of numerical dispersion and it smeares the front.
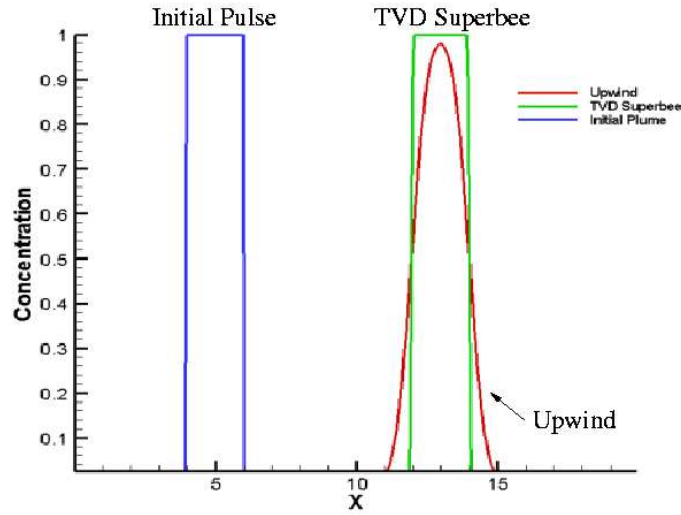

Figure 10: One-dimesional pulse. comparison of upwind and high-resolution TVD FVM.

3.2 Two-dimensional homogeneous

3.2.1 Diagonal uniform velocity field

As the first two-dimensional (2D) test problem, we solved the transport of an initial pulse in a diagonal uniform velocity field. The governing equation of the problem is:

16

$$\frac{\partial c}{\partial t} + \frac{\partial(u_x c)}{\partial x} + \frac{\partial(u_y c)}{\partial y} = 0 \qquad (x, y) \in [0, 1] \times [0, 1], \quad t > 0$$

with initial condition:

$$c_0 = 1 \qquad (x, y) \in (0, 0.12) \times (0, 0.12)$$

The velocity vector $u = (u_x, u_y)$ has a magnitude 1 and it is oriented 45 degrees respect to the x axis. The domain is a square of 1x1 divided in 60x60 elements/cell. The time discretization is $\Delta t = 0.0025$. We simulate a total of 300 time steps. Figure (11) show the inital pulse and the distribution of concentration after 200 time steps. As in the previous example, the first-order method FVM-upwind gives a very poor aproximation of the true solution[6]. Second order method FVM-Superbee produces a much better approximation. We also observe that there is an effect caused by the orientation of the velocity field with respect to the mesh/grid in both methods. However, this effect is much smaller when high-order methods (FVM-Superbee) are used.
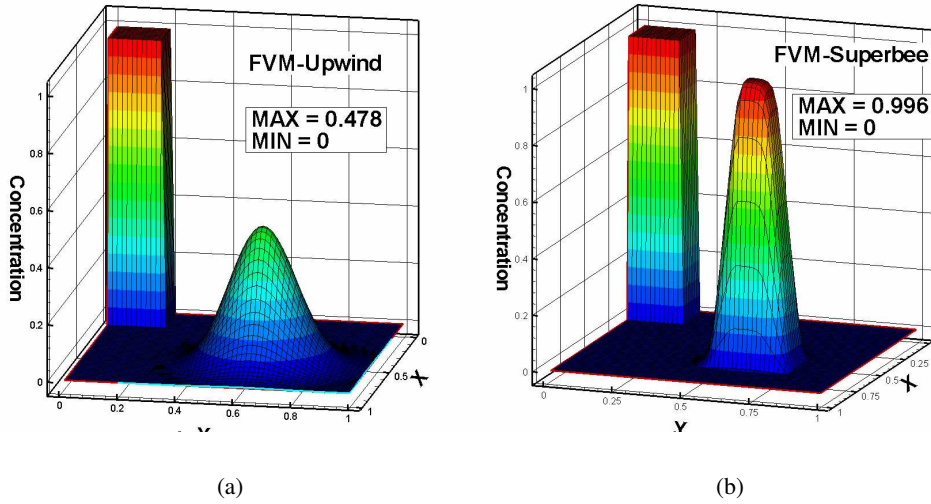

(a)   (b)

Figure 11: Two-dimensional uniform diagonaly oriented velocity field.

3.2.2 Circular velocity field

As a second multidimensional test we used the classical rotating-prism problem (Brooks and Hughes, 1982; Cirpka, 1999). This problem is set by an initial pulse of concentration in a circular velocity field as shown in Figure (12). The main objective of this problem is to compare the concentration after a complete rotation. To set the parameters of the problem we followed

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[6]The true solution is the initial pulse displaced in the diagonal direction: $c(x, y, \Delta t) = c(x - u_x \Delta t, y - u_y \Delta t)$

the description given by Cirpka (1999). We use an angular velocity, $\Omega = 1/10$ [1/s] and a time step $\Delta t = 0.01$ [s] to keep the CFL number under the stability limit. We simulate a total of 1000 time steps that is the time of one rotation. We simulate a square domain of 1x1 discretized into 50x50 elements/cells. The initial pulse/prism of concentration is defined as a square of 5x5 cells where $c = 1$.
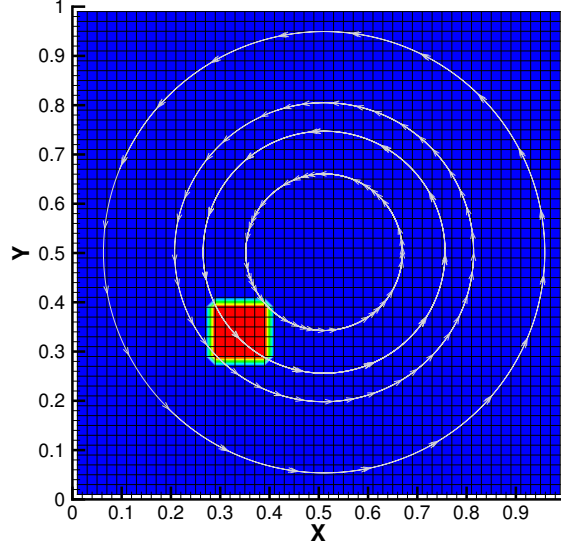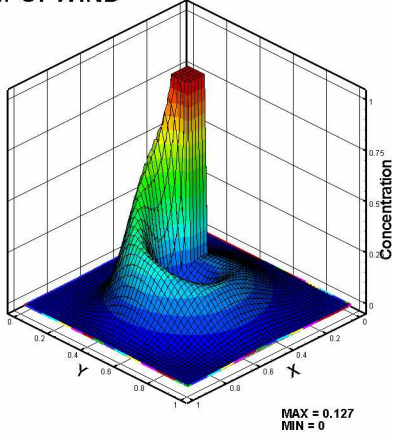

Figure 12: Definition of rotating Prism problem.

Figure (13) shows the solution of this problem given by FVM first-order upwind and second-order Superbee limiter. The first order method FVM-Upwind introduces so much numerical dispersion that the initial pulse has almost vanished after the first rotation. Second order method (FVM-Superbee) avoids an important part of the numerical dispersion of the pure upwind-methods. However, the maximum value of the solution is more than 20% less than the initial value. That means that there still is an important degradation of the numerical solution. Numerical dispersion cannot be avoided even though HRFVM are used.

3.3 Two-dimensional heterogeneous media

As a final test problem we considered a non-uniform velocity field. We used a velocity field generated from a stream-function $\psi(x, y)$ gbibg(Valocchi et al., 2003; Herrera, 2003).
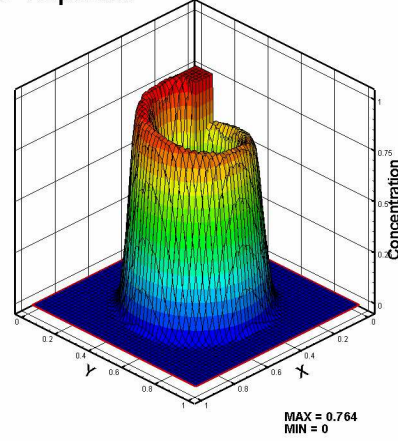
We use a rectangular domain of 1x1 divided into 50x50 elements/cells. We used a time discretization $\Delta t = $1E-3. We simulated a total time equivalent to 1200 time-steps. As the initial

FVM-UPWIND   **FVM- Superbee**

MAX = 0.127
MIN = 0

MAX = 0.764
MIN = 0

(a)   (b)

Figure 13: Comparison of solution for the rotating prism problem. Evolution of the solution during one rotation.

condition we set concentration $c = 1$ in a rectangular region. Figure (14) shows streamlines that define the velocity field and the initial condition of the problem.
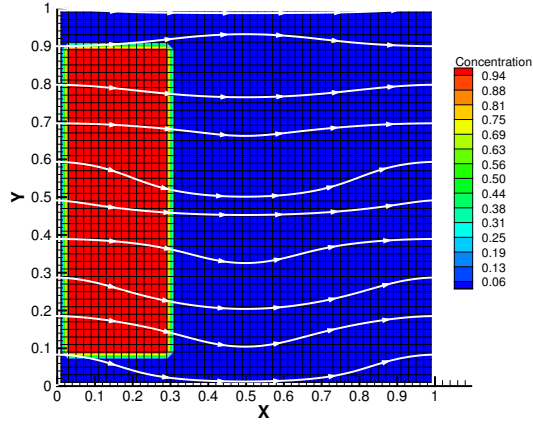

Figure 14: Non-uniform velocity field.

Figure (15) shows the concentration profile after 500 time steps. As expected, high-order FVM gives a better solution than the upwind-FVM . It is interesting to notice that the FVM

19

conserves the initial front/shock, and it seems to give a very good solution for this particular problem. The solution given by the upwind method is completely polluted by numerical dispersion and is a very poor approximation of the actual solution.
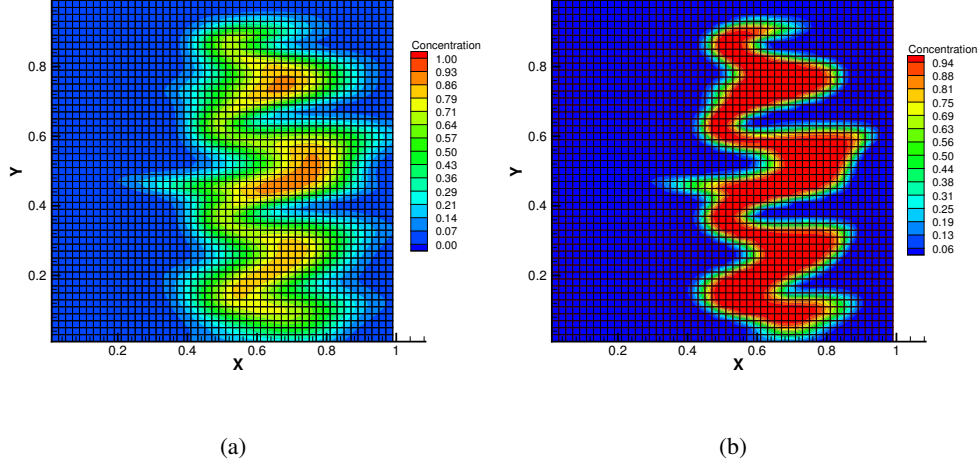

Figure 15: Comparison of solutions for a non-uniform velocity field. a) FVM-Upwind. b) High-resolution FVM-Superbee.

4 Conclusions

Combination of one-dimensional high-resolution TVD methods and the *Fractional-Step* or *Directional-Splitting* (DS) approach proved to be a very powerful alternative for the solution of the conservation law that describes advective transport in heterogeneous porous media. In particular, this approach avoids spurious oscillations giving positive solutions, and at the same time achieves higher accuracy than traditional upwind methods.

For those reasons, the combined use of explict TVD to solve the advective transport and implicit methods to solve the dispersive transport in an Operator-Splitting (OS) approach seems a promising alternative to traditional numerical methods in order to provide a satisfactory solution of the transport term in reactive-transport models solved over Cartesian grids. However, the use of high-resolution finite volume and TVD flux limiters for the solution of complex long-term geochemical process presents a serious challege. In that case, the use of an Operator -Splitting approach is not an option because it introduces unacceptable errors in the solution (Hammond, 2003; Kanney et al., 2003b, a). Fully coupled approaches based on implicit-time approximations have been identified as the best alternative for that case. Those methods make impossible the use of explicit time-marching schemes for temporal integration of the TVD-like high-resolution FVM. The use of implicit TVD methods requires the solution of a non-linear system that must

be solved through iterative Newton-Raphson methods. It is still not clear if the efficiency of those methods will allow the application of implicit-TVD methods to realistic-scale problems. Thus, we recommend these methods as a good choice for the solution of multidimensional non-reactive transport and reactive transport problems where it is possible to use relatively small time steps.

A second topic related to TVD-FVM is the analysis of their practical use in multidimensional problems. As shown above, the DS approach is an easy and inexpensive way to apply the TVD concept to produce monotonic solutions in multidimensions. However, the solution provided by this method is only first-order accurate like any other TVD solution in two or more dimensions (LeVeque, 2002). The use of *Total Variation Bounded in the Mean* (TVBM) limiters in multidimensional scenarios, as applied by Cockburn et al. (1990), is an option that should be explored in more detail. Moreover, the use of advanced unsplit methods or Discontinuous Galerkin FEM for the solution of multidimensional reactive-transport problems might be better alternatives to the DS approach.

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