Preserving bounded and conservative solutions of transport in 1D shallow-water flow with upwind numerical schemes: Application to fertigation and solute transport in rivers

J. Burguete¹, P. García-Navarro²,* and J. Murillo²

¹ Suelo y Agua. Estación Experimental Aula Dei. CSIC. Zaragoza. Spain
² Fluid Mechanics. CPS. University of Zaragoza. Zaragoza. Spain

SUMMARY

This work is intended to show that conservative upwind schemes based on a separate discretization of the scalar solute transport from the shallow water equations are unable to preserve uniform solute profiles in situations of 1D unsteady subcritical flow. However, the coupled discretization of the system is proved to lead to the correct solution in first order approximations. This work is also devoted to show that, when using a coupled discretization, a careful definition of the flux limiter function in second order TVD schemes is required in order to preserve uniform solute profiles. The work shows that, in cases of subcritical irregular flow, the coupled discretization is necessary but nevertheless not enough to ensure concentration distributions free from oscillations and a way to avoid these oscillations is proposed. Examples of steady and unsteady flow in test cases, river and irrigation are presented.

*Correspondence to: pigar@unizar.es

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1. INTRODUCTION

The prediction of solute mixing occurring along a stream of water is important in many applications such as environmental or fertigation studies. The diffuse or the point release of a substance in water is transported with the flow leading to a solute concentration distribution affecting in different form at different distances downstream from the input. The mechanics of mixing is complex and, consequently, practical problems are tackled using a number of assumptions and simplifications. In the most general problem, advection and turbulent diffusion occur in each of the three coordinate directions. However, in cases where a one-dimensional flow model is justified, such as river or channel flow, a tracer originating from a non-steady point source eventually mixes across the channel due to velocity gradients and turbulence and in the far-field a cross sectional averaged concentration can be defined not subject to vertical and transverse concentration gradients. The fate of this cross section averaged tracer concentration is then governed by a one-dimensional advection-dispersion equation [1, 2].

The dynamics of the one-dimensional flow and solute concentration can be studied by means of a system of conservation laws that requires appropriate numerical methods. In the last decades, shock-capturing finite volume schemes of different orders of accuracy for shallow water equations based on approximate Riemann solvers and well balanced to properly incorporate the influence of bed variations and friction terms have been successfully reported [3, 4, 5, 6].
The correct extension of those techniques to include the advection-dispersion equation as well is the main goal of this work.

To obtain an accurate solution of the advective part of the transport process, a non-diffusive numerical scheme is required. To satisfy this requirement some authors have used semi-Lagrangian schemes [7, 8, 9]. This option is linked to a decoupled discretization in which the flow is solved using a different technique. An alternative is to use Eulerian schemes of the appropriate order for the separate system of equations [10, 11, 12]. Furthermore, Eulerian schemes can also be applied to the coupled set of equations [13]. The two last options are analysed in this work.

A one-dimensional shallow-water model including solute transport is formulated both forming a coupled and a decoupled system of equations. It is necessary as a first requirement to evaluate to what extent numerical schemes are able to preserve uniform initial solute profiles in irregular geometries or unsteady flow conditions. As a second goal, a suitable conservative scheme must be able to ensure bounded concentration values. It is not a trivial task since the solute concentration is not one of the conserved variables in our equations system. Several upwind finite volume techniques are presented and a few options considered for their numerical resolution.

The advection-diffusion of a gaussian profile with analytical solution is used as a test case to evaluate the performance of all the schemes discussed. Next the ideal dambreak unsteady flow with uniform solute concentration and with solute discontinuity are used to evaluate the ability of the methods to preserve good properties in the solute distributions. Furthermore, a dambreak flow over sloping and rough bed is used to evaluate the ability of the numerical schemes and approximations to advect an initial square pulse of concentration. Two practical
applications of solute transport, unsteady flow and solute transport on an impervious irrigation border and pollutant spill in a river, are finally presented.

2. FLOW AND TRANSPORT EQUATIONS

The one-dimensional system formed by the cross sectional averaged liquid mass conservation, momentum balance in main stream direction and solute transport can be expressed in conservation form as

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}^c}{\partial x} + \frac{\partial \mathbf{D}}{\partial x} = \mathbf{S}^c,
\]

(1)

where \( \mathbf{U} \) is the vector of conserved variables, \( \mathbf{F}^c \) the flux vector, \( \mathbf{S}^c \) the source term vector, and \( \mathbf{D} \) stands for diffusion

\[
\mathbf{U} = \begin{pmatrix} A \\ Q \\ As \end{pmatrix}, \quad \mathbf{F}^c = \begin{pmatrix} Q \\ gI_1 + \frac{\beta Q^2}{A} \\ Qs \end{pmatrix}, \quad \mathbf{S}^c = \begin{pmatrix} 0 \\ g[I_2 + A(S_0 - S_f)] \\ 0 \end{pmatrix},
\]

\[
\mathbf{D} = \begin{pmatrix} 0 \\ 0 \\ -KA \frac{\partial s}{\partial x} \end{pmatrix},
\]

(2)

with \( A \) the wetted cross section, \( Q \) the discharge, \( s \) the cross sectional average solute concentration, \( g \) the gravity constant, \( S_0 \) the longitudinal bottom slope, \( S_f \) the longitudinal friction slope, \( K \) the diffusion coefficient, \( I_1 \) and \( I_2 \) represent pressure forces

\[
I_1 = \int_0^h (h - z)b \, dz, \quad I_2 = \int_0^h (h - z) \frac{\partial b}{\partial x} \, dz,
\]

(3)
with \( h \) the water depth, \( b \) the cross section width, and \( \beta \) a coefficient resulting from the cross sectional averaging of the velocity

\[
\beta = \frac{A}{Q^2} \int_A v_x^2 \, dA,
\]

with \( v_x \) the longitudinal component of the velocity at any point of the cross section. From the average definition, \( \beta \geq 1 \). When the flow velocity can be considered uniform in the cross section, as in all the examples presented in this work, \( \beta \approx 1 \). However, in cases of irregular or compound cross sections it is known that \( \beta \) can reach values considerably larger so that a model for the velocity distribution in the cross section must be used as in [14, 15].

The friction slope is widely modelled by means of the Gauckler-Manning law [16, 17]

\[
S_f = \frac{n^2 Q |Q|^\frac{3}{4}}{A^{\frac{1}{4}}},
\]

with \( P \) the cross sectional wetted perimeter and \( n \) the Gauckler-Manning roughness coefficient. The diffusion coefficient contains all the information related to molecular or viscous diffusion, turbulent diffusion and dispersion derived from the cross sectional and turbulent averaging process. The model proposed by Rutherford [2] will be used

\[
K = 10 \sqrt{gPA|S_f|}.
\]

The system of equations can be expressed in non-conservative form taking into account

\[
\frac{dF^c(x, U)}{dx} = \frac{\partial F^c}{\partial x} + J \frac{\partial U}{\partial x},
\]

with \( J \) the flux Jacobian

\[
J = \frac{\partial F^c}{\partial U} = \begin{pmatrix}
0 & 1 & 0 \\
c^2 - \beta u^2 & 2\beta u & 0 \\
-us & s & u
\end{pmatrix},
\]
where $u = Q/A$ is the cross sectional average velocity, $c = \sqrt{gA/B}$ is the velocity of the infinitesimal waves and $B$ is the cross section top width. Inserting in (1)

$$\frac{\partial U}{\partial t} + J \frac{\partial U}{\partial x} + \frac{\partial D}{\partial x} = S^{nc},$$

(9)

with $S^{nc}$ the non-conservative source term

$$S^{nc} = S^c - \frac{\partial F^c}{\partial x} = \begin{pmatrix} 0 \\ c^2 \frac{\partial A}{\partial x} - Au^2 \frac{\partial \beta}{\partial x} - gA \left( \frac{\partial z_s}{\partial x} + S_f \right) \\ 0 \end{pmatrix},$$

(10)

where $z_s$ is the water surface level.

The Jacobian matrix can be made diagonal

$$J = P \Lambda P^{-1}, \quad P = \begin{pmatrix} 1 & 1 & 0 \\ \lambda_1 & \lambda_2 & 0 \\ s & s & 1 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

(11)

with $\Lambda$ the eigenvalues diagonal matrix, $P$ the diagonalizer matrix and $\lambda_i$ the Jacobian eigenvalues corresponding to the characteristic propagation celerities

$$\lambda_1 = \beta u + \sqrt{c^2 + (\beta^2 - \beta)u^2}, \quad \lambda_2 = \beta u - \sqrt{c^2 + (\beta^2 - \beta)u^2}, \quad \lambda_3 = u.$$  

(12)

The eigenvalues are related to the flow regime

- $\lambda_1 \lambda_2 > 0 \Rightarrow \beta u^2 > c^2 \Rightarrow$ Supercritical flow.
- $\lambda_1 \lambda_2 < 0 \Rightarrow \beta u^2 < c^2 \Rightarrow$ Subcritical flow.

By defining the differential characteristic variables $dW$ as

$$dW = P^{-1} dU,$$

(13)

and left-multiplying the non-conservative equation (9) by $P^{-1}$ the characteristic differential equations are obtained

$$\frac{\partial W}{\partial t} + \Lambda \frac{\partial W}{\partial x} + P^{-1} \frac{\partial D}{\partial x} = P^{-1} S^{nc}.$$  

(14)
A last, simple and very convenient form of the equations is the quasi-conservative form. Taking into account that
\[
\frac{dI_1}{dx} = I_2 + A \frac{dz_s}{dx},
\] (15)
and inserting in (1)
\[
\frac{\partial U}{\partial t} + \frac{\partial F^{qc}}{\partial x} + \frac{\partial D}{\partial x} = S^{qc},
\] (16)
with \( F^{qc} \) and \( S^{qc} \) the quasi-conservative flux and source terms
\[
F^{qc} = \begin{pmatrix}
Q \\
\frac{a g^2}{A} \\
Q_s
\end{pmatrix}, \quad S^{qc} = \begin{pmatrix}
0 \\
-g A \left( \frac{dz_s}{dx} + S_f \right) \\
0
\end{pmatrix},
\] (17)
It must be stressed that, under the form (16), the equations do not furnish the correct propagation information. The Jacobian matrix of the quasi-conservative form is
\[
J^{qc} = \frac{\partial F^{qc}}{\partial U} = \begin{pmatrix}
0 & 1 & 0 \\
-\beta u^2 & 2 \beta u & 0 \\
-u s & s & u
\end{pmatrix},
\] (18)
with the eigenvalues
\[
\lambda_1 = \left( \beta + \sqrt{\beta^2 \beta} \right) u, \quad \lambda_2 = \left( \beta - \sqrt{\beta^2 \beta} \right) u, \quad \lambda_3 = u,
\] (19)
that do not correspond to the characteristic celerities of propagation of the information in this medium as in (12).

3. SEPARATE DISCRETIZATION OF THE SOLUTE TRANSPORT EQUATION

The simplest and most common way to solve the system of equations (2) is to discretize the mass and momentum flow equations separately, in each time step, from the solute...
transport equation. Letting aside the method applied to the flow equations, let us consider the conservative form of the transport equation

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \]  

being \( U = As \) the conserved variable and \( F = uAs - KA \frac{\partial s}{\partial x} \) the flux. This flux can be decomposed into a flux \( T \) due to advection and another flux \( D \) due to diffusion. In this case

\[ F = T + D, \quad T = uAs, \quad D = -KA \frac{\partial s}{\partial x}, \]

we shall next concentrate on the description and discussion of different numerical methods suitable for the discretization of this equation alone.

3.1. First order upwind scheme with implicit diffusion

Upwind schemes are based on a spatial discretization according to the sign of the characteristic celerities of propagation in the system. Hence, spatial derivatives are evaluated at every point using a computational cell larger than the correct region of influence of that point. Combining the first order explicit upwind scheme applied to the advection and the centred implicit scheme to solve the diffusion, both in conservative form, the following scheme is obtained

\[ \Delta U_i^n = -\frac{\Delta t}{\delta x} \left[ (\delta T^+_{i-1/2})^n + (\delta T^-_{i+1/2})^n + D^{n+\theta}_{i+1/2} - D^{n+\theta}_{i-1/2} \right], \]  

with \( \delta T^+ \) and \( \delta T^- \) associated to propagation velocities positive and negative respectively

\[ u^\pm = \frac{1}{2} (u \pm |u|), \quad \delta T^\pm = \frac{u^\pm}{u} \delta T, \]

where the notation \( f^{n+\theta} = \theta f^{n+1} + (1 - \theta) f^n \) has been used.

3.2. Second order in space TVD scheme with implicit diffusion

Combining the second order in space TVD explicit scheme applied to the advection and the centred implicit scheme to solve the diffusion, both in conservative form, the following second
order in space TVD semi-implicit scheme is obtained

\[
\Delta U^n_i = -\frac{\Delta t}{\delta x} \left\{ \left( \delta T^+ \right)_{i-(1/2)}^n + \left( \delta T^- \right)_{i+(1/2)}^n + D^{n+\theta}_{i+(1/2)} - D^{n+\theta}_{i-(1/2)} + \frac{1}{2} \left[ \left( \Psi^+ \delta T^+ \right)_{i-(1/2)}^n \right. \right.
\]

\[
- \left. \left( \Psi^+ \delta T^+ \right)_{i-(3/2)}^n + \left( \Psi^- \delta T^- \right)_{i+(1/2)}^n - \left( \Psi^- \delta T^- \right)_{i+(3/2)}^n \right\}, \tag{24}
\]

where \( \Psi^+ \) and \( \Psi^- \) are the flux limiter functions which are defined to combine the second order spatial centred and upwind schemes, to preserve the second order and, according to the (100) properties, to avoid the numerical oscillations. In order to produce a second order scheme, the dependence of flux limiter functions is defined as follows [21]

\[
\Psi^+_{i+(1/2)} = \Psi \left( \frac{\delta T^+_{i+(3/2)}}{\delta T^+_{i+(1/2)}} \right), \quad \Psi^-_{i+(1/2)} = \Psi \left( \frac{\delta T^-_{i-(1/2)}}{\delta T^-_{i+(1/2)}} \right). \tag{25}
\]

3.3. Second order in space and time TVD scheme with implicit diffusion

By combining the Sweby second order in space and time TVD explicit scheme [18] applied to the advection and the centred implicit scheme to solve the diffusion, both in conservative form, the following scheme is obtained

\[
\Delta U^n_i = -\frac{\Delta t}{\delta x} \left\{ \left( \delta T^+ \right)_{i-(1/2)}^n + \left( \delta T^- \right)_{i+(1/2)}^n + D^{n+\theta}_{i+(1/2)} - D^{n+\theta}_{i-(1/2)} + \frac{1}{2} \left[ \left( \Psi^+ \delta E^+ \right)_{i-(1/2)}^n \right. \right.
\]

\[
- \left. \left( \Psi^+ \delta E^+ \right)_{i-(3/2)}^n + \left( \Psi^- \delta E^- \right)_{i+(1/2)}^n - \left( \Psi^- \delta E^- \right)_{i+(3/2)}^n \right\}, \tag{26}
\]

with

\[
\delta E^\pm = (1 \mp \sigma) \delta T^\pm, \quad \sigma = u \frac{\Delta t}{\delta x}, \quad \sigma^\pm = \frac{1}{2} (\sigma \pm |\sigma|). \tag{27}
\]

It is worth signalling that, although this scheme is named second order in space and time, this is not strictly true since it is not second order in time for the diffusion term. The dependence of the flux limiter functions is defined as [21]

\[
\Psi^+_{i+(1/2)} = \Psi \left( \frac{(\delta E^+)^n_{i+(3/2)}}{(\delta E^+)^n_{i+(1/2)}} \right), \quad \Psi^-_{i+(1/2)} = \Psi \left( \frac{(\delta E^-)^n_{i-(1/2)}}{(\delta E^-)^n_{i+(1/2)}} \right). \tag{28}
\]
4. COUPLED DISCRETIZATION OF THE SYSTEM

In what follows, our interest will be focused in the analysis of the discretization of the coupled system of equations using the most efficient techniques from section 3: the first order upwind and the second order in space and time TVD. Despite the apparently unnecessary extra complexity of this approach, it will prove the only way to improve the accuracy of the numerical solution in many cases, as previously reported [13].

4.1. First order upwind scheme with implicit diffusion

According to the form of the scheme based on the characteristic form (87), the following decomposition matrices are defined

$$
\Phi^\pm = \begin{pmatrix}
\phi_1^\pm & 0 & 0 \\
0 & \phi_2^\pm & 0 \\
0 & 0 & \phi_3^\pm
\end{pmatrix},
$$

(29)

and, at the same time, the upwind matrices associated to the propagation directions:

$$
\phi_i^\pm = \frac{1}{2}[1 \pm \text{sign}(\lambda_i)], \quad \Omega^\pm = \Phi^\pm \Phi^{-1}, \quad G^\pm = \Omega^\pm G.
$$

(30)

In order to deal with transcritical problems in which the flow passes from subcritical to supercritical, the introduction of an artificial viscosity like the one proposed by Harten-Hyman [19] is necessary. This scheme becomes

$$
\Delta U_i^n = \Delta t \left[ (G^+ - \nu \frac{\delta U}{\delta x})_{i-(1/2)} + (G^- + \nu \frac{\delta U}{\delta x})_{i+(1/2)} - \frac{1}{\delta x} (D_{i+\theta}^{n+\theta} - D_{i-\theta}^{n-\theta}) \right],
$$

(31)

with $\nu$ an artificial viscosity coefficient defined as in [20]

$$
\nu_{i+(1/2)}^n = \max_k \left\{ \frac{1}{4} [\delta(\lambda_k) - 2|\lambda_k|]_{i+(1/2)}, \quad \text{if } (\lambda_k)_i^n < 0 \text{ and } (\lambda_k)_{i+1}^n > 0 \right\}.
$$

(32)
Note that, for supercritical flow, $\Omega^- = 1$, $\Omega^+ = 0$ and this discretization is identical to (22). The same is not true for subcritical flow.

We shall postulate that the TVD condition for this combined scheme is governed by the most restrictive among the different eigenvalues, that is
\begin{equation}
0 \leq \theta \leq 1, \quad \Delta t \leq \min \left[ \frac{\delta x}{|\beta u| + \sqrt{(\beta^2 - \beta)u^2 + c^2}}, \frac{\delta x^2}{|u|\delta x + (1 - \theta)2K} \right].
\end{equation}

4.2. Second order in space and time TVD scheme with implicit diffusion

The simplest form to extend the described scalar second order in space and time TVD scheme (26) to the coupled system of equations is
\begin{equation}
\Delta U^n_i = \Delta t \left\{ \left( G^+ - \nu \frac{\delta U}{\delta x} \right)_{i-1/2}^n + \left( G^- + \nu \frac{\delta U}{\delta x} \right)_{i+1/2}^n - \frac{1}{\delta x} \left( D^n_{i+1/2}^{n+\theta} - D^n_{i-1/2}^{n+\theta} \right) \right. \\
+ \frac{1}{2} \left[ (\Psi^+ E^+)_{i-1/2}^n - (\Psi^+ E^+)_{i+1/2}^n + (\Psi^- E^-)_{i-1/2}^n - (\Psi^- E^-)_{i+1/2}^n \right] \left. \right\},
\end{equation}
with the second order vectors
\begin{equation}
E^\pm = \left(1 \mp J \frac{\Delta t}{\delta x}\right) G^\pm.
\end{equation}
The flux limiting matrices are defined as
\begin{equation}
\Psi^\pm_{i+1/2} = \begin{pmatrix}
\Psi \left( \frac{(E^\pm)^{i+1/2} + 1}{(E^\pm)^{i+1/2}} \right) & 0 & 0 \\
0 & \Psi \left( \frac{(E^\pm)^{i+1/2} + 1}{(E^\pm)^{i+1/2}} \right) & 0 \\
0 & 0 & \Psi \left( \frac{(E^\pm)^{i+1/2} + 1}{(E^\pm)^{i+1/2}} \right)
\end{pmatrix},
\end{equation}
with $(E^\pm)^i$ the $i$ component of vector $E^\pm$. This new form of defining the flux limiting matrices, based on the components of the second order vector, will be called vectorial limiting discretization.

Another alternative is to define the second order vectors as
\begin{equation}
L^\pm = \left(1 \mp \Lambda \frac{\Delta t}{\delta x}\right) P^{-1} G^\pm.
\end{equation}
Then, the second order in space and time TVD scheme is written as

\[
\Delta U^n_i = \Delta t \left\{ \left( G^+ - \nu \frac{\delta U}{\delta x} \right)_{i-(1/2)}^n + \left( G^- + \nu \frac{\delta U}{\delta x} \right)_{i+(1/2)}^n - \frac{1}{\delta x} \left( D^+_{i+(1/2)} - D^-_{i-(1/2)} \right) \right. \\
+ \frac{1}{2} \left[ \left( P \Psi^+ L^+ \right)^n_{i-(1/2)} - \left( P \Psi^+ L^+ \right)^n_{i-(3/2)} + \left( P \Psi^- L^- \right)^n_{i+(1/2)} - \left( P \Psi^- L^- \right)^n_{i+(3/2)} \right] \right\},
\]

(38)

and the flux limiting matrices are

\[
\Psi_{i+(1/2)}^\pm = \begin{pmatrix}
\Psi \left( \frac{L^+_{i+(1/2)+1}}{L^+_{i+(1/2)}} \right) & 0 & 0 \\
0 & \Psi \left( \frac{L^+_{i+(1/2)+1}}{L^+_{i+(1/2)}} \right) & 0 \\
0 & 0 & \Psi \left( \frac{L^+_{i+(1/2)+1}}{L^+_{i+(1/2)}} \right)
\end{pmatrix}
\]

(39)

This second form of defining the flux limiting matrices, more in the line of the characteristic form of the scheme (86), will be named characteristic limiting discretization.

Using that in the scalar case the TVD conditions for this scheme are identical to those for the first order scheme, we shall postulate that this scheme is TVD whenever (33) holds.

5. PRESERVING BOUNDED SOLUTIONS SCHEMES

5.1. Preserving initial uniformity schemes

When the initial concentration as well as the boundary conditions are uniform, \( \frac{\partial s}{\partial x} = 0 \), the third of the conservation equations (1) becomes

\[
\frac{\partial (As)}{\partial t} + \frac{\partial (Qs)}{\partial x} = \frac{\partial}{\partial x} \left( KA \frac{\partial s}{\partial x} \right) = 0.
\]

(40)

By developing the derivatives and using the mass conservation equation

\[
A \frac{\partial s}{\partial t} + s \left( \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} \right) = 0 \Rightarrow \frac{\partial s}{\partial t} = 0,
\]

(41)
indicating that, under these conditions, the concentration must stay constant in time whatever the flow conditions. A numerical scheme unable to reproduce this important property will be unacceptable.

This case will be solved using the first order upwind scheme with decoupled discretization, that is, solving in every time step first the system of mass and momentum flow equations (two first components of equation system (31)) and, separately, (22). With \( \theta = 0 \) and assuming positive discharges

\[
\begin{pmatrix}
A^n_{i+1} \\
Q^n_{i+1}
\end{pmatrix}
= \begin{pmatrix}
A^n_i \\
Q^n_i
\end{pmatrix}
- \Delta t \left\{ \begin{pmatrix}
\Omega^{+} \frac{\delta}{\delta x} \left( \begin{pmatrix}
Q^n_i \\
H^n_i
\end{pmatrix}
\right)
\end{pmatrix}_{i+(1/2)}
+ \begin{pmatrix}
\Omega^{-} \frac{\delta}{\delta x} \left( \begin{pmatrix}
Q^n_i \\
H^n_i
\end{pmatrix}
\right)
\end{pmatrix}_{i-(1/2)} \right\},
\]

\((As)^{n+1}_i = (As)^n_i - \frac{\Delta t}{\delta x} \left[ (Qs)^n_i - (Qs)^n_{i-1} \right] + \frac{1}{\delta x} \left[ \left( KA \frac{\delta s}{\delta x} \right)^n_{i+1/2} - \left( KA \frac{\delta s}{\delta x} \right)^n_{i-1/2} \right], \quad (42)\)

where, in order to simplify the notation, the following has been defined:

\[
\frac{\delta H}{\delta x} = gA \left( \frac{\delta z_s}{\delta x} + S_f \right) + \frac{\delta}{\delta x} \left( \frac{\beta Q^2}{A} \right).
\]

With uniform concentration initial conditions \( s^n_i = \text{const.} = s_0 \)

\[
A^n_{i+1} s^{n+1}_i = A^n_i s_0 - s_0 \frac{\Delta t}{\delta x} (Q^n_i - Q^n_{i-1}). \quad (44)
\]

In this case the diagonalizer matrix is

\[
P = \begin{pmatrix}
1 & 1 \\
\lambda_1 & \lambda_2
\end{pmatrix}.
\]

For supercritical flow \( \Omega^+ = 1, \Omega^- = 0 \) so that

\[
A^n_{i+1} = A^n_i - \frac{\Delta t}{\delta x} (Q^n_i - Q^n_{i-1}), \quad s^{n+1}_i = s_0,
\]

therefore, the scheme is able to keep uniform the concentration for unsteady supercritical flows.
However, in the case of subcritical flow

\[
\Omega^+ = P \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} P^{-1} = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix} -\lambda_2 & 1 \\ -\lambda_1 \lambda_2 & \lambda_1 \end{pmatrix},
\]

\[
\Omega^- = P \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} P^{-1} = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix} \lambda_1 & -1 \\ \lambda_2 \lambda_1 & -\lambda_2 \end{pmatrix},
\]

so that

\[
A_i^{n+1} = A_i^n - \frac{\Delta t}{\delta x} \left[ \left( \frac{-\lambda_2 \delta Q + \delta H}{\lambda_1 - \lambda_2} \right)^n_{i-\frac{1}{2}} + \left( \frac{\lambda_1 \delta Q - \delta H}{\lambda_1 - \lambda_2} \right)^n_{i+\frac{1}{2}} \right],
\]

\[
s_i^{n+1} = \frac{A_i^n - \frac{\Delta t}{\delta x} \left( Q_i^n - Q_i^{n-1} \right)}{A_i^n - \frac{\Delta t}{\delta x} \left( \frac{-\lambda_2 \delta Q + \delta H}{\lambda_1 - \lambda_2} \right)^n_{i-\frac{1}{2}} + \left( \frac{\lambda_1 \delta Q - \delta H}{\lambda_1 - \lambda_2} \right)^n_{i+\frac{1}{2}}} S_0.
\]

Hence, in a general case, it cannot be said that \( s_i^{n+1} = s_0 \) and the scheme, although conservative and stable, produces a distortion in the uniform concentration distribution for unsteady subcritical flow. This is a non-trivial handicap for conservative schemes using decoupled discretization of the transport equation.

If the first order upwind scheme is applied to the coupled system (31) with \( \theta = 0 \), assuming positive discharge and uniform concentration initial conditions

\[
\begin{pmatrix} A \\ Q \\ A_s \end{pmatrix}_{i}^{n+1} = \begin{pmatrix} A \\ Q \\ A_s \end{pmatrix}_{i}^{n} - \Delta t \left\{ \begin{pmatrix} \Omega^n \frac{\delta}{\delta x} \begin{pmatrix} Q \\ H \end{pmatrix} \\ T \end{pmatrix}_{i-\frac{1}{2}}^{n} + \Omega^n \frac{\delta}{\delta x} \begin{pmatrix} Q \\ H \end{pmatrix} \\ T \end{pmatrix}_{i+\frac{1}{2}}^{n} \right\}.
\]

In this case, \( P \) is defined as in (11). For supercritical flow \( \Omega^+ = 1, \Omega^- = 0 \) so that

\[
A_i^{n+1} = A_i^n - \frac{\Delta t}{\delta x} \left( Q^n_i - Q^n_{i-1} \right), \quad s_i^{n+1} = s_0,
\]

and the scheme reproduces the uniform concentration during the unsteady calculation.
Preserving bounded and conservative solutions of transport

Subcritical flow

\[
\Omega^+ = P \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} P^{-1} = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix} \lambda_1 - 1 & 0 \\ -\lambda_2 \lambda_2 & \lambda_1 - 0 \\ -\lambda_1 s & s \lambda_1 - \lambda_2 \end{pmatrix},
\]

\[
\Omega^- = P \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} P^{-1} = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix} \lambda_1 - 0 & 0 \\ \lambda_1 \lambda_2 & -\lambda_2 - 0 \\ \lambda_1 s & -s - 0 \end{pmatrix},
\]

so that

\[
A_{i+1}^n = A_i^n - \frac{\Delta t}{\delta x} \left[ \left( \frac{-\lambda_2 \delta Q + \delta H}{\lambda_1 - \lambda_2} \right)_{i-(1/2)} + \left( \frac{\lambda_1 \delta Q - \delta H}{\lambda_1 - \lambda_2} \right)_{i+(1/2)} \right],
\]

\[
s_{n+1}^i = \frac{A_{i+1}^n}{A_i^n} \left[ \left( \frac{-\lambda_2 \delta Q + \delta H + (\lambda_1 - \lambda_2)\delta T}{\lambda_1 - \lambda_2} \right)_{i-(1/2)} + \left( \frac{\lambda_1 \delta Q - \delta H}{\lambda_1 - \lambda_2} \right)_{i+(1/2)} \right],
\]

\[
s_0 = s_0,
\]

and the scheme is also able to guarantee uniform concentration during the unsteady calculation.

It is easy to show that this also occurs when using the TVD schemes with characteristic limiting discretization (38). However, the vectorial limiting discretization (34) does not guarantee that the scheme preserves uniformity in the transported scalar distribution, see Fig. 7. Hence, even though it might seem an unnecessary complication in the procedure, the coupled formulation of the system of equations and the characteristic limiting discretization are crucial to improve the quality of the solutions in unsteady solute transport problems.
5.2. Preserving bounded solution schemes

A little transformation in the conservative transport equation that involves the use of the mass conservation equation, leads to the characteristic form of the transport equation:

$$\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} = 1 \frac{\partial}{\partial x} \left( K A \frac{\partial s}{\partial x} \right).$$  \hfill (53)

In absence of diffusion ($K = 0$) this is an scalar wave equation

$$\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} = 0,$$  \hfill (54)

with exact solution given an initial solute distribution $s_0(x)$, representing the pure advection

$$s(x, t) = s_0 \left( x - \int_0^t u(x', t')dt' \right), \quad \frac{dx'}{dt'} = u(x', t').$$  \hfill (55)

Therefore, the solution of the equation contains the same extrema in concentration that are present in the initial conditions. The numerical schemes that have the property of being able to preserve this condition will be called ”preserving bounded solution” schemes. Obviously, the methods which do not preserve a uniform concentration are neither able to meet these new property.

Given, for instance, a discontinuous initial concentration distribution with uniform values at both sides of the discontinuity as represented in Fig. 1. If a numerical scheme that preserves

Figure 1. Discontinuous solute concentration distribution with a jump between nodes $i$ and $i+1$. 

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bounded solution is sought, it must hold

\[ s_i^n \geq s_i^{n+1} \geq s_{i+1}^n, \quad s_i^n \geq s_i^{n+1} \geq s_{i+1}^{n+1}. \]  

(56)

We shall first consider the first order upwind scheme with coupled discretization in order to study whether it meets (56). For supercritical flow \((G^+ = G, G^- = 0)\) in this case

\[
A_i^{n+1} = A_i^n - \frac{\Delta t}{\delta x} \delta Q_{i-(1/2)}^n, \quad (As)_{i}^{n+1} = (As)_{i}^n - \frac{\Delta t}{\delta x} \delta (Qs)_{i-(1/2)}^n,
\]

\[
A_{i+1}^{n+1} = A_{i+1}^n - \frac{\Delta t}{\delta x} \delta Q_{i+(1/2)}^n, \quad (As)_{i+1}^{n+1} = (As)_{i+1}^n - \frac{\Delta t}{\delta x} \delta (Qs)_{i+(1/2)}^n.
\]

(57)

Taking into account that

\[ s_i^{n-1} = s_i^{n-(1/2)} = s_i^n \geq s_{i+1}^n = s_i^{n+(3/2)} = s_i^{n+2}, \]

(58)

working out the solute concentrations in (57)

\[ s_i^{n+1} = s_i^n, \quad s_i^{n+1} = \frac{(As)_{i}^{n+1} - \frac{\Delta t}{\delta x} [(Qs)_{i+1}^n - (Qs)_{i}^n]}{A_{i+1}^n - \frac{\Delta t}{\delta x} \delta Q_{i+(1/2)}^n}. \]

(59)

This solution meets (56) since

\[
s_i^{n+1} = \frac{(As)_{i}^{n+1} - \frac{\Delta t}{\delta x} [(Qs)_{i+1}^n - (Qs)_{i}^n]}{A_{i+1}^n - \frac{\Delta t}{\delta x} \delta Q_{i+(1/2)}^n} \leq \frac{(As)_{i}^n - \frac{\Delta t}{\delta x} [(Qs)_{i+1}^n - (Qs)_{i}^n]}{A_{i+1}^n - \frac{\Delta t}{\delta x} \delta Q_{i+(1/2)}^n} = s_i^{n+1},
\]

\[
s_i^n \geq s_i^{n+1} \Leftrightarrow s_i^n \left( A_{i+1}^n - \frac{\Delta t}{\delta x} \delta Q_{i+(1/2)}^n \right) \geq (As)_{i+1}^n - \frac{\Delta t}{\delta x} [(Qs)_{i+1}^n - (Qs)_{i}^n] \Leftrightarrow
\]

\[
s_i^n \left( A - \frac{\Delta t}{\delta x} Q_{i+1}^n \right) \geq \left( A - \frac{\Delta t}{\delta x} Q_{i+1}^n \right) s_i^n \Leftrightarrow u_{i+1}^n \frac{\Delta t}{\delta x} \leq 1,
\]

(60)

and this holds whenever the scheme stability condition (33) holds.

In cases of subcritical flow an artificial diffusion will be added to the first order upwind scheme with coupled discretization so that even in absence of physical diffusion the following
decomposition will be applied:

\[ G_{i+1/2}^L = [G^+ - V]_{i+1/2}, \quad G_{i+1/2}^R = [G^- + V]_{i+1/2}, \quad V = -\frac{1}{\delta x} \begin{pmatrix} 0 \\ 0 \\ \xi \delta s \end{pmatrix} \text{,} \]

with \( \xi \) an strictly positive \((\xi \geq 0)\) artificial diffusion coefficient. We shall next state the conditions over this parameter for the scheme to meet \((56)\). Applying the scheme to our problem

\[
A_i^{n+1} = A_i^n - \frac{\Delta t}{\delta x} [(\delta Q^+)_i^{n-1/2} + (\delta Q^-)_i^{n+1/2}],
\]

\[
A_{i+1}^{n+1} = A_{i+1}^n - \frac{\Delta t}{\delta x} [(\delta Q^+)_i^{n+1/2} + (\delta Q^-)_i^{n+3/2}],
\]

\[
(As)_i^{n+1} = (As)_i^n - \frac{\Delta t}{\delta x} [\delta(Qs)_i^{n-1/2} - (s\delta Q^- - \xi s)_i^{n+1/2} + (s\delta Q^- - \xi s)_i^{n+1/2}],
\]

\[
(As)_{i+1}^{n+1} = (As)_{i+1}^n - \frac{\Delta t}{\delta x} [\delta(Qs)_{i+1/2} - (s\delta Q^- - \xi s)_{i+1/2} + (s\delta Q^- - \xi s)_{i+1/2}],
\]

where, for the sake of simplicity in the notation, the following has been used

\[
\delta Q^+ = -\frac{\lambda_2\delta Q + \delta H}{\lambda_1 - \lambda_2}, \quad \delta Q^- = \frac{\lambda_1\delta Q - \delta H}{\lambda_1 - \lambda_2}.
\]

Taking into account that

\[
[\delta(Qs) - s\delta Q^-]_{i+1/2} = (Q\delta s + s\delta Q - s\delta Q^-)_{i+1/2} = (Q\delta s + s\delta Q^+)_{i+1/2},
\]

using \((58)\) and working out the concentrations:

\[
s_i^{n+1} = \frac{(As)_i^n - \frac{\Delta t}{\delta x} [s_i^n \delta(Q^+)_i^{n-1/2} + (s\delta Q^- - \xi s)_i^{n+1/2}]}{A_i^n - \frac{\Delta t}{\delta x} [(\delta Q^+)_i^{n-1/2} + (\delta Q^-)_i^{n+1/2}]},
\]

\[
s_{i+1}^{n+1} = \frac{(As)_{i+1}^n - \frac{\Delta t}{\delta x} [(Q\delta s)_{i+1/2} + (s\delta Q^+ + \xi s)_{i+1/2} + s_{i+1}^{n+1} \delta(Q^-)_i^{n+3/2}]}{A_{i+1}^n - \frac{\Delta t}{\delta x} [(\delta Q^+)_i^{n+1/2} + (\delta Q^-)_i^{n+3/2}]},
\]
Inserting these expressions in the conditions (56) the inequalities hold provided that

\[
\xi^n_{i+1/2} \geq (\delta Q^-)^n_{i+1/2} \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i}, \quad \xi^n_{i+1/2} \geq -Q^n_{i+1/2} + (\delta Q^+)_{i+1/2}^n \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i},
\]

\[
\Delta t \leq \frac{A_i^{n+1} \delta x}{\xi^n_{i+1/2} - (\delta Q^-)_{i+1/2}^n \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i}}.
\]

\[
\Delta t \leq \frac{A_i^{n+1} \delta x}{\xi^n_{i+1/2} + Q^n_{i+1/2} - (\delta Q^+)_{i+1/2}^n \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i}}.
\]

Hence, the artificial diffusion coefficient can be defined:

\[
\xi^n_{i+1/2} = \begin{cases} 
\max \left[ 0, (\delta Q^-)^n_{i+1/2} \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i} \right], & \text{if } \beta u^2 < c^2 \\
-Q^n_{i+1/2} + (\delta Q^+)_{i+1/2}^n \frac{s^n_{i+1} - s^n_i}{s^n_{i+1} - s^n_i}, & \text{if } \beta u^2 \geq c^2
\end{cases}
\]

(67)

Using this, the right hand side quantities in the two last inequalities (66) are strictly positive, so that the scheme can meet all the necessary conditions to preserve the bounded solution by reducing the time step if necessary. It can also be proved that the same conditions keep also bounded a solution with the opposite sign in the discontinuity, that is:

\[
s_i^n \leq s_i^{n+1} \leq s_i^{n+1}, \quad s_i^n \leq s_i^{n+1} \leq s_i^{n+1}.
\]

(68)

Since a series of discontinuities is a typical spatial approximation in a discretization, the above conditions can be considered sufficient to keep bounded any initial distribution.

Given that the second order in space and time TVD scheme reduces to the first order upwind scheme in the vicinity of discontinuities the same artificial diffusion coefficient will be applied. Then, using for instance the characteristic limiting discretization of the flux limiter, the scheme with artificial diffusion is

\[
\Delta U^n_i = \Delta t \left\{ \left( G^+ - \frac{\delta U}{\delta x} - V \right)_{i-(1/2)}^n + \left( G^- + \frac{\delta U}{\delta x} + V \right)_{i+(1/2)}^n \right\}
\]
\[
\frac{1}{\delta x} \left( D_{n+\theta}^{n+(1/2)} - D_{n-\theta}^{n-(1/2)} \right) \\
+ \frac{1}{2} \left\{ \left( P\Psi^{+}L^{+} \right)_{i-(1/2)}^{n} - \left( P\Psi^{+}L^{+} \right)_{i-(3/2)}^{n} + \left( P\Psi^{-}L^{-} \right)_{i+(1/2)}^{n} - \left( P\Psi^{-}L^{-} \right)_{i+(3/2)}^{n} \right\}. \tag{69}
\]

6. BOUNDARY CONDITIONS

A correct numerical model for unsteady flow problems must be based not only on a conservative and accurate numerical scheme but also on an adequate procedure to discretize the boundary conditions. The theory of characteristics provides clear indications about the number of necessary external boundary conditions to define a well posed problem [21].

For the water flow, two external physical boundary conditions are required at the inlet and two numerical boundary conditions are required at the outlet in cases of supercritical flow; however, both a physical and a numerical boundary condition at the inlet and at the outlet are necessary in cases of subcritical flow. The most usual physical boundary conditions at the inlet are a discharge hydrograph \( Q(t) \) or a water depth limnigraph \( h(t) \) in case of subcritical flow and both together \( Q(t), h(t) \) in case of supercritical flow. At the outlet, the most common practices to use are a rating curve of the type \( Q = Q(h) \) or a limnigraph \( h(t) \).

Critical outlet or closed outlet can be considered particular cases. For the solute transport, a physical boundary condition at the inlet, being a concentration input \( s(t) \) the most usual, and a numerical boundary condition at the outlet are required.

The method of global mass conservation [22, 23] is based on enforcing the integral form of the mass conservation extended to all the computational domain in combination with a conservative scheme for the interior points to generate the numerical boundary condition. In a domain discretized using \( N \) cells, if a conservative scheme defined by a nodal flux \( F^T \) is used...
all over the domain, the cross section increments predicted in one time step are
\[ \Delta A^n_i = -\frac{\Delta t}{\delta x} \left( \delta Q^R_{i-(1/2)} + \delta Q^L_{i+(1/2)} \right), \quad \Delta (As)^n_i = -\frac{\Delta t}{\delta x} \left( \delta T^R_{i-(1/2)} + \delta T^L_{i+(1/2)} \right). \] (70)

Therefore, the total numerical water volume \( \Delta V^n \) and solute mass \( \Delta M^n \) variations produced by the scheme are, neglecting contributions from outside cells (\( \delta F^L_{i/2} = \delta F^R_{N+1/2} = 0 \))
\[ \Delta V^n = \sum_{i=1}^{N} \Delta A^n_i \delta x = -\Delta t \sum_{i=1}^{N} \left( \delta Q^L_{i-(1/2)} + \delta Q^R_{i+(1/2)} \right) = \Delta t \left( Q^T_1 - Q^T_N \right), \]
\[ \Delta M^n = \sum_{i=1}^{N} \Delta (As)^n_i \delta x = -\Delta t \sum_{i=1}^{N} \left( \delta T^L_{i-(1/2)} + \delta T^R_{i+(1/2)} \right) = \Delta t \left( T^T_1 - T^T_N \right). \] (71)

Since the scheme used is conservative, the variations are only due to the boundaries and can be split into numerical contributions at the inlet and at the outlet in the following form
\[ \Delta V^n = \Delta V^n_{\text{in}} + \Delta V^n_{\text{out}}, \quad \Delta V^n_{\text{in}} = \Delta t Q^T_1, \quad \Delta V^n_{\text{out}} = -\Delta t Q^T_N, \]
\[ \Delta M^n = \Delta M^n_{\text{in}} + \Delta M^n_{\text{out}}, \quad \Delta M^n_{\text{in}} = \Delta t T^T_1, \quad \Delta M^n_{\text{out}} = -\Delta t T^T_N. \] (72)

If the physical boundary condition are, for instance, a certain water volume \( \Delta V^{phy} \) or solute mass \( \Delta M^{phy} \) inputs at the inlet or at the outlet, in order to ensure the global mass conservation of the scheme the numerical mass increments must be corrected. This is achieved by means of additional increments \( \Delta A \) and \( \Delta (As) \) at the inlet or at the outlet, that must be added to those previously obtained by the numerical scheme (70), so that
\[ \Delta V^{phy}_{\text{in}} = \Delta A^a_1 \delta x + \Delta t Q^T_1, \quad \Delta V^{phy}_{\text{out}} = \Delta A^a_N \delta x - \Delta t Q^T_N, \]
\[ \Delta M^{phy}_{\text{in}} = \Delta (As)^a_1 \delta x + \Delta t T^T_1, \quad \Delta M^{phy}_{\text{out}} = \Delta (As)^a_N \delta x - \Delta t T^T_N. \] (73)

Since all the schemes considered meet \( F^T_i = (F^c)^n_i \), the additional increments are
\[ \Delta A^a_1 = \frac{\Delta V^{phy}_{\text{in}} - \Delta t Q^T_1}{\delta x}, \quad \Delta A^a_N = \frac{\Delta V^{phy}_{\text{out}} + \Delta t Q^T_N}{\delta x}, \]
\[ \Delta (As)^a_1 = \frac{\Delta M^{phy}_{\text{in}} - \Delta t (Qs)^T_1}{\delta x}, \quad \Delta (As)^a_N = \frac{\Delta M^{phy}_{\text{out}} + \Delta t (Qs)^T_N}{\delta x}. \] (74)

More details on the use of these conditions in different particular cases can be found in [23].
7. ANALYTICAL SOLUTIONS TO THE ADVECTION-DIFFUSION EQUATION

7.1. Advection-diffusion of a gaussian profile

There are cases where the advection-diffusion equation can be solved analytically. This cases are very useful to validate the numerical solutions. Considering constant the cross-sectional area, the velocity and the diffusion coefficient, the linearised equation is

\[
\frac{\partial s}{\partial t} + u \frac{\partial s}{\partial x} = K \frac{\partial^2 s}{\partial x^2}.
\]  

(75)

With an initial gaussian profile, analytical solutions to this equation can be obtained

\[
s(x, t) = s_0 + \frac{s_1}{\sqrt{1 + 4aKt}} \exp \left[ -a(x - x_0 - ut)^2 \right].
\]

(76)

We shall first consider a case of pure diffusion of a profile with \(s_0 = 0.2Kg/m^3\), \(s_1 = 0.6Kg/m^3\), \(a = 0.04m^{-2}\), \(u = 0m/s\), \(K = 0.2m^2/s\) and \(x_0 = 50m\) after 250 seconds, as represented in Fig. 2(a), and the propagation of a profile with \(s_0 = 0.1Kg/m^3\), \(s_1 = 0.8Kg/m^3\), \(a = 0.01m^{-2}\), \(u = 1m/s\), \(K = 0.2m^2/s\) and \(x_0 = 20m\) after 60 seconds, as represented in Fig. 2(b). To simulate the profiles, a grid with \(\Delta x = 1m\) will be used. The numerical results for the pure

![Figure 2. (a) Pure diffusion and (b) advection-diffusion of a gaussian profile.](image-url)
diffusion case, shown in Fig. 3, indicate that the explicit scheme is the most accurate for the diffusion. The implicit scheme with \( \theta = 1 \) presents a slight antidiffusive tendency that becomes more noticeable as the time step size increases. The numerical antidiffusivity decreases with the parameter \( \theta \) although, for large time steps, the TVD criterion can be violated in this case and numerical oscillations may appear (Fig. 3(d)). In order to simultaneously avoid numerical oscillations and minimise the antidiffusivity, in what follows the smallest value of \( \theta \) compatible with the TVD conditions (105) and (107) will be used:
First order and second order in space and time TVD with implicit diffusion schemes

\[ \theta = \max \left[ 0, 1 - \left( \frac{\delta x}{\Delta t} - |u| \right) \frac{\delta x}{2K} \right]. \] (77)

Second order in space TVD with implicit diffusion scheme

\[ \theta = \max \left\{ 0, 1 - \left[ \frac{\delta x}{\Delta t} - |u| \left( 1 + \frac{1}{2} \max(\Psi) \right) \right] \frac{\delta x}{2K} \right\}. \] (78)

With these definitions for \( \theta \) the time step size restrictions due to diffusion are eliminated and the Courant-Friedrichs-Lewy CFL number is defined as

\[ \Delta t = CFL \min_i \left[ \frac{\delta x}{\beta|u| + \sqrt{c^2 + (\beta^2 - \beta)|u|^2}} \right]^n. \] (79)

Fig. 4 is a plot of the advection-diffusion results. It can be seen that, for the first order upwind scheme, the antidiffusivity of the implicit discretization of the diffusion counterbalances the numerical diffusion inherent to the first order advection scheme leading to an acceptable result. However, the antidiffusivity adds up with the antidiffusivity inherent to the second order in space TVD scheme, producing results of worse quality than the first order approach, specially with the "Superbee" limiter. If, at the same time, the increased complexity and reduced size of the time steps required by this scheme are considered, it can be discarded for transport problems. On the other hand, the second order in space and time TVD scheme provides the most accurate results, almost independently of the flux limiter used, with a slight diffusive tendency using the "Minmod" function and a slight antidiffusive tendency when using the "Superbee" limiter.

7.2. Ideal dambreak with uniform solute concentration and with solute discontinuity

The ideal dambreak problem is one of the classical examples used as test cases for unsteady shallow water flow simulations. The reason is that for flat and frictionless bottom, rectangular
Figure 4. Advection-diffusion of a gaussian profile using the schemes: (a) 1st order upwind explicit, (b) 2nd order in space TVD and (c) 2nd order in space and time TVD with different time step sizes. In (a), (b) and (c) $\Delta t = 0.5s$ is used.

cross section and no diffusion, the problem defined by zero initial velocity and initial discontinuities in the water depth and solute concentration has an exact solution [24].

A rectangular channel 200$m$ long and 1$m$ wide has been considered with an initial depth ratio 1$m : 0.1m$. A grid spacing of $\delta x = 2m$ and $CFL = 0.9$ was used for all the simulations. The plots in Fig. 5 show the numerical solution for the water depth from three schemes versus the exact solution for $t = 20s$.

A second case corresponds to the same dambreak discontinuity together with a uniform
Figure 5. Ideal dambreak depth with the schemes of (a) 1st order upwind, (b) and (c) 2nd order in space and time TVD with different flux limiters ((b) “Minmod” and (c) “Superbee”).

initial solute concentration of 1*Kg/m^3*. Fig. 6 displays the concentration results for *t = 20s* using the separated discretization. None of the numerical schemes is able to keep the concentration uniform as time progresses. Fig. 7 shows the results obtained with the coupled discretization for the same test case. The first order upwind scheme preserves the uniform concentration as well as the second order TVD scheme with different flux limiters if the characteristic limiting formulation is used. When the vectorial limiting discretization is used for the limiters, the numerical solution is not free from oscillations.

As a third dambreak test case, an initial discontinuity in the concentration of 1*Kg/m^3*: 


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Figure 6. Ideal dambreak concentration with the separated discretization and the schemes of (a) 1st order upwind, (b) and (c) 2nd order in space and time TVD with different flux limiters ((b) "Minmod" and (c) "Superbee").

0 Kg/m³ in the same location as the depth jump has been considered. Fig. 8 shows the results obtained at \( t = 2 \) s using the coupled discretization with and without the artificial diffusion described in section 7. It is clear that without the artificial diffusion slight numerical oscillations appear near the front and that they disappear when using artificial diffusion. Fig. 9 shows the results provided by the schemes using the coupled discretization, artificial diffusion and characteristic limiting discretization for \( t = 20 \) s. The first order scheme produces more numerical damping than the second order schemes as expected. Among the limiting functions,
Figure 7. Ideal dambreak concentration with the coupled discretization and the schemes of (a) 1st order upwind, (b), (c), (d) and (e) 2nd order in space and time TVD with (b) and (c) characteristic, (d) and (e) vectorial limiting discretization; (b) and (d) "Minmod", (c) and (e) "Superbee" flux limiter.
Figure 8. Ideal dambreak discontinuous concentration for $t = 2s$ with the coupled discretization with and without artificial diffusion and the characteristic limiting discretization for the (a) 1st order upwind and the 2nd order in space and time schemes with the flux limiter (b) "Minmod" and (c) "Superbee".

"Superbee" appears slightly more accurate than "Minmod".
8. PRACTICAL APPLICATIONS

8.1. Flow and solute transport on an impervious irrigation border

The experimental data from [12] were used to validate the proposed models in cases of steady and unsteady flow in conditions of high relative roughness. In that experiment a free-draining irrigation border 200 m long and 2 m wide, with a slope of $S_0 = 0.000671$ was constructed and covered with plastic film. A fine layer gravel (with $d_{50}$ of approximately 20 mm) was added on top of the plastic film. Two unsteady flow experiments of water flow advancing over the dry border bed were performed and will be simulated for calibration. In case 1, an inlet discharge of $Q = 0.0048 \text{ m}^3/\text{s}$ was applied and, after 1033 s of water application, 7 kg of salt were released during 180 s at the upstream end. The water inlet was interrupted at $t = 2698$ s. In case 2 the inlet discharge was $Q = 0.0118 \text{ m}^3/\text{s}$, 28 kg of salt were released during 360 s and the water inflow was interrupted at $t = 2265$ s. For the bed roughness simulation, a Manning coefficient $n = 0.09 \text{ sm}^{-1/3}$ was used and, for the longitudinal dispersion coefficient the (6) model was adopted. From the computational point of view, a grid with 2000 nodes
was involved, a $CFL = 0.9$ was fixed all the time and the second order in space and time TVD scheme with characteristic limiting discretization, "Superbee" flux limiter and artificial diffusion (69) was applied.

In case 1, 5100s of experiment were simulated and 3900s in case 2. Figs. 10 and 11 show longitudinal profiles of surface level (front advance) and solute concentration respectively at different times for both cases. They are useful to see that the selected numerical method is completely free from numerical oscillations even at the locations close to the advancing front.

![Simulated surface level longitudinal profiles for different times of cases (a) 1 and (b) 2.](image)

![Simulated concentration longitudinal profiles for different times of cases (a) 1 and (b) 2.](image)
Fig. 12 illustrates the good behaviour of the solution in the simulation of the front advance. In both cases, the numerical advance has been compared with the measured advance. Figs. 13 and 14 are comparisons of the time evolution of the measured and calculated concentration at several gauging points for both cases 1 and 2 respectively. The results indicate that the accuracy provided by this scheme is enough for this kind of application. The observed differences can be attributed mostly to the diffusion model, although it is remarkable that the simple Rutherford model, proposed for river mixing with very different flow conditions, provides a reasonable approximation without any fitting procedure. The simulation results are satisfactory since they accurately predict the advancing velocity. However, the model overestimates the dispersion effect mainly in case 2.

8.2. Pollutant spill in a river

In order to show the practical application of the model in a river flow context, a hazardous and instantaneous pollutant spill of 20 T of petrol at a point of a 11.4 km reach of the Ebro River will be simulated. The solubility of the petrol at the typical temperature of the river water was
Figure 13. Measured and simulated time evolution of concentration of case 1 at (a) $x = 50m$, (b) $x = 100m$ and (c) $x = 150m$.

estimated as $0.03Kg/m^3$. For higher concentrations, the petrol was assumed to precipitate to the bottom remaining there. The steady annual base river discharge of $200m^3/s$ was assumed. In a first run, the steady state water surface profile corresponding to that discharge in the river reach was calculated. Fig. 15a represents the bed and surface levels at steady state. The spill was located at $700m$ of the upstream end. Fig. 15b shows two concentration longitudinal profiles at $1h$ and $2h$ of the spill. The Spanish law establishes that $9.5mg/m^3$ is the limit of tolerance for the pernicious influence of petrol concentration in riverine ecological systems. Fig. 15c represents the time evolution of borders of the contaminant cloud with a concentration
Figure 14. Measured and simulated time evolution of concentration of case 2 at (a) $x = 50m$, (b) $x = 100m$ and (c) $x = 150m$.

9. CONCLUSIONS

A conservative formulation of the system of equations governing the water flow and the solute transport has been adopted as the basis of our study. The formulation of several finite volume conservative upwind schemes well suited for the numerical simulation of one-dimensional shallow-water flow and solute transport has been provided. Two possibilities have exceeding the dangerous limit.
Figure 15. Petrol spill in Ebro river: (a) longitudinal bed and water surface profiles, (b) longitudinal concentration profiles at 1h and 2h after the spill, (c) time evolution of the plume of concentration exceeding the dangerous threshold.

been identified, separate or coupled discretization, leading to different degree of influence of the flow processes to the solute transport at the discrete level.

It has been proved that well balanced conservative upwind schemes based on a separate discretization of the scalar solute transport from the shallow water equations are not able to preserve uniform solute profiles in situations of unsteady subcritical flow even when using first order methods. However, the coupled formulation and discretization of the system is proved to lead to the correct solution in first order approximations.
When seeking more accuracy second order TVD schemes can be applied. It has been shown that a careful definition of the flux limiter function is required in order to preserve uniform solute profiles in the solute distribution function in cases of unsteady subcritical flow.

The work shows that, in cases of subcritical unsteady irregular flow, the coupled discretization is necessary but nevertheless not enough to always ensure concentration distributions free from oscillations and a way to use an artificial diffusion in subcritical cases is proposed.

The validation test cases show the good performance of the second order TVD schemes for the coupled system formulation in cases of steady and unsteady flow.

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APPENDIX

I. PROPERTIES OF THE EULERIAN NUMERICAL SCHEMES

I.1. Conservation

The conservative form (1) can be integrated in a time interval $T$ and in a domain length $L$ to
get a global rule of conservation

$$
\int_0^T \int_0^L \left( \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial D}{\partial x} \right) \ dx \ dt = \int_0^L S \ dx \ dt \Rightarrow 
$$

$$
\int_0^L U(x,t) \ dx - \int_0^L U(x,0) \ dx = \int_0^T \left[ F(0,t) + D(0,t) \right] \ dt - \int_0^T \left[ F(L,t) + D(L,t) \right] \ dt 
+ \int_0^T \int_0^L S \ dx \ dt, \quad (80)
$$
telling us that the time variation of the conserved variables is equal to the flux entering minus the flux leaving the system plus the contribution of the source terms. When discretizing a conservation law like (1), bad numerical approximations can lead to unacceptable error.

Schemes approximating the conservation equation (80) correctly are called conservative.
schemes [5]. A definition of a conservative scheme follows the structure proposed by Lax [25]

\[ \Delta U^n_i = \Delta t \left[ S^n_i - \frac{1}{\delta x} \left( F^n_{i+1/2} - F^n_{i-1/2} \right) \right], \quad (81) \]

where \( F^* \) and \( S^* \) are the numerical flux and source term respectively, and represent a suitable approximation to the physical flux and source term. \( \Delta \) will be used for time increments \( \Delta f^n = f^{n+1} - f^n \), and \( \delta \) represents spatial increment \( \delta f_i = f_{i+1} - f_i \). Schemes so defined are conservative since they produce a good approximation of (80), provided that the discretization of fluxes and source terms is consistent, that is

\[ F^* \approx F^c + D, \quad S^* \approx S^c. \quad (82) \]

Adding up all the increments defined by the numerical scheme (81) in a grid of \( N \) spatial nodes and \( M \) time steps, an approximation of the global conservation (80) is obtained

\[
\sum_{j=0}^{M-1} \sum_{i=1}^{N-1} \Delta U^n_i \delta x \approx \int_{x_{1/2}}^{x_{N-(1/2)}} U(x, t^M) \, dx - \int_{x_{1/2}}^{x_{N-(1/2)}} U(x, t^0) \, dx, \\
\sum_{j=0}^{M-1} \sum_{i=1}^{N-1} (S^*)_i \delta x \Delta t \approx \int_{0}^{t^M} dt \int_{x_{1/2}}^{x_{N-(1/2)}} S(x, t) \, dx, \\
- \sum_{j=0}^{M-1} \sum_{i=1}^{N-1} \Delta t \left[ (F^*)_{i+1/2} - (F^*)_{i-1/2} \right] = \sum_{j=0}^{M-1} \Delta t \left[ (F^c)_{N-(1/2)} - (F^c)_{1/2} \right] \\
\approx \int_{t^0}^{t^M} \left[ F^c(x_{1/2}, t) + D(x_{1/2}, t) \right] dt - \int_{t^0}^{t^M} \left[ F^c(x_{N-(1/2)}, t) + D(x_{N-(1/2)}, t) \right] dt. \quad (83)
\]

A numerical flux \( F^T \) can also be defined at the grid nodes. The difference in this flux across a grid cell can be decomposed into incoming and outgoing parts. Schemes so built follow

\[
\delta F^T_{i+1/2} = F^T_{i+1} - F^T_i = \delta F^R_{i+1/2} + \delta F^L_{i+1/2}, \]

\[ \Delta U^n_i = \Delta t \left[ \left( S - \frac{\delta F}{\delta x} \right)_{i-(1/2)}^{L} + \left( S - \frac{\delta F}{\delta x} \right)_{i+(1/2)}^{R} \right]. \quad (84)\]
This also leads to conservative schemes since this form can be shown to be equivalent to (81) and the following interface numerical flux can be defined [5, 6] 

\[ F^*_{i+1/2} = F^T_{i+1/2} - \delta F^L_{i+1/2}, \quad S^*_{i+1/2} = S^T_{i+1/2} + S^R_{i-1/2}. \]  

A conservative scheme can be derived by discretizing the characteristic form of the equations (14) 

\[ \Delta W^n_i = \Delta t \left\{ \Phi^L_{i-(1/2)} \left( P^{-1} S^{nc} - \Lambda \frac{\delta W}{\delta x} \right)_{i-(1/2)} + \Phi^R_{i+(1/2)} \left( P^{-1} S^{nc} - \Lambda \frac{\delta W}{\delta x} \right)_{i+(1/2)} \right. \]
\[ \left. - \frac{P^{-1}}{\delta x} \left(D^R_{i+(1/2)} - D^L_{i-(1/2)} \right) \right\}, \]  

with \( \Phi^L,R_{i+(1/2)} \) the characteristic decomposition matrices. Multiplying back by \( P \) in order to recover the physical variables, extracting \( P^{-1} \) and using (11), (86) can be written 

\[ \Delta U^n_i = \Delta t \left\{ \left[ P \Phi^R P^{-1} \left( S^{nc} - J \frac{\partial U}{\partial x} \right) \right]_{i+(1/2)} + \left[ P \Phi^L P^{-1} \left( S^{nc} - J \frac{\partial U}{\partial x} \right) \right]_{i+(1/2)} \right. \]
\[ \left. - \frac{1}{\delta x} \left(D^R_{i+(1/2)} - D^L_{i-(1/2)} \right) \right\}. \]  

This scheme will be conservative if the following condition at the discrete level is enforced [6] 

\[ (I_2)_{i+(1/2)} = \delta (I_1)_{i+(1/2)} - A_{i+(1/2)} \delta h_{i+(1/2)}, \]
\[ u_{i+1/2} = \frac{\sqrt{A_{i+1} u_{i+1} + \sqrt{A_i} u_i} + \sqrt{A_i} u_i}{\sqrt{A_{i+1}}}, \quad s_{i+1/2} = \frac{\sqrt{A_{i+1} s_{i+1} + \sqrt{A_i} s_i} + \sqrt{A_i} s_i}{\sqrt{A_{i+1}} + \sqrt{A_i}}. \]  

In order to complete the formulation, the choice of some average values remains open. The simplest option has been used in this work 

\[ A_{i+1/2} = \frac{A_{i+1} + A_i}{2}, \quad \beta_{i+1/2} = \frac{\beta_{i+1} + \beta_i}{2}, \quad C_{i+1/2} = \sqrt{\frac{A_{i+1} + A_i}{B_{i+1} + B_i}}. \]
The conservative decomposition matrices will be defined as

\[ \Omega^{R,L} = P \Phi^{R,L} P^{-1}, \quad \Omega^{R} + \Omega^{L} = \Phi^{R} + \Phi^{L} = 1. \quad (91) \]

By defining, at the same time, the vectors

\[ G^{R,L} = \Omega^{R,L} G, \quad (92) \]

the non-conservative, quasi-conservative and conservative forms of this scheme can be written as follows

\[ \Delta U^n_{i} = \Delta t \left[ G^{R}_{i+1/2} + G^{L}_{i-1/2} - \frac{1}{\delta x} \left(D^{R}_{i+1/2} - D^{L}_{i-1/2}\right)\right]. \quad (93) \]

Since the three forms are equivalent, the simplest quasi-conservative is recommended [6].

The considered numerical schemes are conservative since it’s admit the following wave decomposition:

- First order upwind scheme with implicit diffusion

\[ F^{T}_{i} = (F^{c})_{i}^{n}, \quad G^{L}_{i+1/2} = \left(G^{+} - \nu \frac{\delta U}{\delta x}\right)_{i+1/2}^{n} + \frac{1}{\delta x} D^{n+\theta}_{i+1/2}, \]

\[ G^{R}_{i+1/2} = \left(G^{-} + \nu \frac{\delta U}{\delta x}\right)_{i+1/2}^{n} - \frac{1}{\delta x} D^{n-\theta}_{i+1/2}. \quad (94) \]

- Second order in space and time TVD scheme with implicit diffusion and vectorial limiting discretization

\[ F^{T}_{i} = (F^{c})_{i}^{n}, \]

\[ G^{L}_{i+1/2} = \left(G^{+} - \nu \frac{\delta U}{\delta x}\right)_{i+1/2}^{n} - \frac{1}{2} \left(\Psi^{+} E^{+}\right)_{i-(1/2)}^{n} + \frac{1}{2} \left(\Psi^{-} E^{-}\right)_{i-(3/2)}^{n} + \frac{1}{\delta x} D^{n+\theta}_{i+1/2}, \]

\[ G^{R}_{i+1/2} = \left(G^{-} + \nu \frac{\delta U}{\delta x}\right)_{i+1/2}^{n} + \frac{1}{2} \left(\Psi^{+} E^{+}\right)_{i-(1/2)}^{n} - \frac{1}{2} \left(\Psi^{-} E^{-}\right)_{i-(3/2)}^{n} - \frac{1}{\delta x} D^{n+\theta}_{i+1/2}. \quad (95) \]

- Second order in space and time TVD scheme with implicit diffusion and characteristic limiting discretization

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\[ F^T_i = (F^-)_i^n, \]
\[ G^L_{i+(1/2)} = \left( G^+ - \nu \frac{\partial U}{\partial x}_{i+(1/2)} \right)^n - \frac{1}{2} \left( P\Psi^+ L^+ \right)^n_{i-(1/2)} + \frac{1}{2} \left( P\Psi^- L^- \right)^n_{i+(3/2)} + \frac{1}{\delta x} D^{n+\theta}_{i+(1/2)}, \]
\[ G^R_{i+(1/2)} = \left( G^- + \nu \frac{\partial U}{\partial x}_{i+(1/2)} \right)^n + \frac{1}{2} \left( P\Psi^+ L^+ \right)^n_{i-(1/2)} - \frac{1}{2} \left( P\Psi^- L^- \right)^n_{i+(3/2)} - \frac{1}{\delta x} D^{n+\theta}_{i+(1/2)}. \]

**I.2. TVD property**

A general three-point scheme, applied to a scalar advection-diffusion equation, can be expressed like

\[ \Delta U^n_i + A^- \delta U^{n+1}_{i+(1/2)} + A^+ \delta U^{n+1}_{i-(1/2)} = B^- \delta U^n_{i+(1/2)} + B^+ \delta U^n_{i-(1/2)}. \]

Even though linear stability and numerical dissipation prevent any amplification of the perturbations, they do not remove completely oscillations from the numerical solution. The Total Variation Diminishing property was defined to meet this goal. Starting from the definition of the “Total Variation” of a numerical solution as

\[ TV^n = \sum_i \left| \delta U^n_{i+(1/2)} \right|, \]

a numerical scheme is said to be TVD (“Total Variation Diminishing”) if

\[ TV^{n+1} \leq TV^n. \]

Sufficient conditions (although not necessary) ensuring that a general scheme like (97) applied to the linear scalar equation is TVD are

\[ A^- \leq 0, \quad A^+ \geq 0, \quad B^- \geq 0, \quad B^+ \leq 0, \quad B^- - B^+ \leq 1. \]

An unstable scheme cannot be TVD.

Making a linearised analysis, with \( A, K \) and \( u \) constants, the following coefficients of the general scheme (97) can be defined for the considered schemes

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• First order upwind scheme with implicit diffusion

\[
A^+ = \theta \frac{K \Delta t}{\delta x^2}, \quad A^- = -\theta \frac{K \Delta t}{\delta x^2}, \quad B^+ = -\frac{u^+ \Delta t}{\delta x} - (1-\theta) \frac{K \Delta t}{\delta x^2}, \quad B^- = -\frac{u^- \Delta t}{\delta x} + (1-\theta) \frac{K \Delta t}{\delta x^2}.
\] (101)

• Second order in space TVD scheme with implicit diffusion

\[
A^+ = \theta \frac{K \Delta t}{\delta x^2}, \quad A^- = -\theta \frac{K \Delta t}{\delta x^2},
\]

\[
B^+_{i+1/2} = - \left[ 1 + \frac{1}{2} \left( \Psi^+(r) \right)_{i+1/2} - \frac{1}{2} \left( \frac{\Psi^+ \delta T^+}{\delta x} \right)_{i+1/2} \right] \frac{u^+ \Delta t}{\delta x} - (1-\theta) \frac{K \Delta t}{\delta x^2},
\]

\[
B^-_{i+1/2} = - \left[ 1 + \frac{1}{2} \left( \Psi^-(r) \right)_{i+1/2} - \frac{1}{2} \left( \frac{\Psi^- \delta T^-}{\delta x} \right)_{i+1/2} \right] \frac{u^- \Delta t}{\delta x} + (1-\theta) \frac{K \Delta t}{\delta x^2}.
\] (102)

• Second order in space and time TVD scheme with implicit diffusion

\[
A^+ = \theta \frac{K \Delta t}{\delta x^2}, \quad A^- = -\theta \frac{K \Delta t}{\delta x^2},
\]

\[
B^+_{i+1/2} = - \left[ 1 + \frac{1}{2} \left( 1 - \sigma \right)_{i+1/2} \left( \Psi^+(r) \right)_{i+1/2} - \frac{1}{2} \left( \frac{\Psi^+ \delta E^+}{\delta x} \right)_{i+1/2} \left( \sigma^+ \right)_{i+1/2} - \right. \\
\left. - (1-\theta) \frac{K \Delta t}{\delta x^2} \right]
\]

\[
B^-_{i+1/2} = - \left[ 1 + \frac{1}{2} \left( 1 + \sigma \right)_{i+1/2} \left( \Psi^-(r) \right)_{i+1/2} - \frac{1}{2} \left( \frac{\Psi^- \delta E^-}{\delta x} \right)_{i+1/2} \left( \sigma^- \right)_{i+1/2} + \right. \\
\left. + (1-\theta) \frac{K \Delta t}{\delta x^2} \right].
\] (103)

Applying the TVD conditions (100) to second order in space TVD scheme with implicit diffusion, the flux limiter will be a positive function so that

\[
\Psi(r) = 0, \ \forall r < 0; \quad \Psi(r) \leq 2r, \ \forall r > 0,
\] (104)

and this leads to the following conditions

\[
0 \leq \theta \leq 1, \quad \Delta t \leq \frac{\delta x^2}{\left[ \frac{1}{2} \max(\Psi) \right] u |\delta x + (1-\theta)2K}.
\] (105)
It is usual to establish the restriction $\Psi(r) \leq 2$ in order to be able to work with time step sizes up to $\Delta t \leq \frac{\delta x}{2|u|}$. The intersection between the second order region and the TVD region for the flux limiter functions in the second order in space TVD scheme is represented in Fig. 16.

Many particular flux limiter functions are defined in previous works [26, 27, 28]. We use the extreme values:

- "Superbee" [26]: $\Psi(r) = \max\{0, \min(1, 2r), \min(2, r)\}$
- "Minmod" [26]: $\Psi(r) = \max\{0, \min(1, r)\}$

Applying the TVD conditions (100) to second order in space and time TVD scheme with implicit diffusion, the flux limiter will be a positive function so that

$$\Psi(r) = 0, \forall r < 0; \quad \Psi(r) \leq 2r, \forall r > 0; \quad \Psi(r) \leq 2, \forall r. \quad (106)$$

The intersection between the second order region and the TVD region for the flux limiter functions in the second order in space and time TVD scheme is identical to the second order in space TVD region, being Fig. 16 and the flux limiter functions defined are also valid for this scheme. Applying conditions (100) to first order upwind and second order in space and time TVD schemes with implicit diffusion, both are TVD for

$$0 \leq \theta \leq 1, \quad \Delta t \leq \frac{\delta x^2}{|u|\delta x + (1 - \theta)2K}. \quad (107)$$