Stability Criterion for Explicit Schemes (Finite-Difference Method) on the Solution of the Advection-Diffusion Equation

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Abstract

The numerical solutions of the advection-diffusion equation are themselves numerous and sometimes very sophisticated, in order to avoid two undesirable features: oscillatory behavior and numerical diffusion. It is known that the common practice of "splitting-up" the solution is not always the best approach to the advection-diffusion problem. By using the ordinary differential equation analogy method (Aldama , 1987), this paper develops a stability criterion for theexplicit first order central scheme, for solving the advection-diffusion equation in its linear steady flow form.

This formulation of the stability analysis presents the stability criterion as a function of both local Courant and Péclét numbers. In order to show the features of the stability criterion proposed, comparisons between analytical solutions and those obtained with the schemes are presented for the classical one-dimensional semi-infinite problem with initial and boundary conditions of continuous discharge of pollutant. Applying the stability criterion found in this paper, the finite difference explicit scheme results are very satisfactory.

Introduction

Due to the wide range of types of water pollutants, from something as harmless as organic wastes to deathly chemicals, environmental strategies must rely on the knowledge of the process involved in the evolution of the concentration produced by the dispersion of the substance to be disposed of. The general idea that "dilution is the solution to pollution" is, besides a simplistic one, just suitable for some organic materials which are to be reassimilated in the global ecosystem.

Among the studies of transport processes, there are three great categories: those related to improve the understanding of the physical basis of the process, the ones which deals with numerical techniques in the simulation of contaminant dispersion, and those in which the efforts are centered in the validation of both by means of calibration with physical models and field data. This paper is a contribution in the aspects of computational simulation of the dispersion process.

The most general statement of conservation of contaminant mass in a control volume subject to advective and diffusive flux across its boundaries is (Fischer et al., 1979):

$$\frac{\partial C}{\partial t} + \vec{V} \cdot \nabla C = D\nabla^2 C \qquad (1)$$

where C(x,y,z,t) = contaminant concentration, V(x,y,z,t) = instantaneous vector velocity at a point, and D=molecular diffusivity. Equation (1) assumes incompressible ambient fluid, and adopts Fick's law of simple proportionality between diffusive contaminant flux and the concentration gradient.

The longitudinal dispersion process can be described by a bulk one-dimensional dispersion equation averaged over time and space. Replacing the molecular diffusivity D by a longitudinal dispersion coefficient K (Taylor, 1954), and writing equation (1) in its one-dimensional form as:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial x^2} \qquad (2)$$

An explicit method of solution

To solve the above expression, known as the one-dimensional dispersion equation, the finite-difference approximations (Smith, 1977) were used and replaced in equation (2) to write a general form of an explicit first order scheme as:

$$C_i^{n+1} = A_0 C_{i-1}^n + A_1 C_i^n + A_2 C_{i+1}^n \qquad (3)$$

with the values of the coefficients given in Table 1.

Table 1. *Coefficients of first order explicit scheme*

Scheme	A_0	A_1	A_2
Backward	λ + Cr	1 - 2λ - Cr	λ
Central	λ + Cr/2	1 - 2λ	λ - Cr/2
Forward	λ	1 - 2λ + Cr	λ - Cr

where Cr is the Courant number, Pe is the local Péclét number, and lamda is the ratio between them.

Stability analysis

After surveying the relevant literature on the subject, we discovered that no practical stability criterion exists for (3). This finding was surprising, in view of the simplicity that such scheme has. It is known that some numerical approximations of equation (2) produce spurious oscillations and numerical diffusion when advection dominates.

It is a common practice to split-up the equation into two parts, for pure advection and pure diffusion perform the stability analysis for each separate equations, and then use the combined criterion in the solution of the complete dispersion equation.

The stability criteria for the separate forms of equation (2) are well known, Abbot (1979) & Smith (1977), and stands that when using forward-difference approximations in time and space the scheme for pure advection is stable and free from numeric diffusion when Cr<=1, and in the other hand, lamda<=1/2 as the condition for pure diffusion problems.

Results of the numerical solution with the complete scheme (3), using the conditions given above, are compared with the analytical solution (see section 'Comparing solutions') in figure 1, showing the oscillatory behavior and the overshooting of the solution.

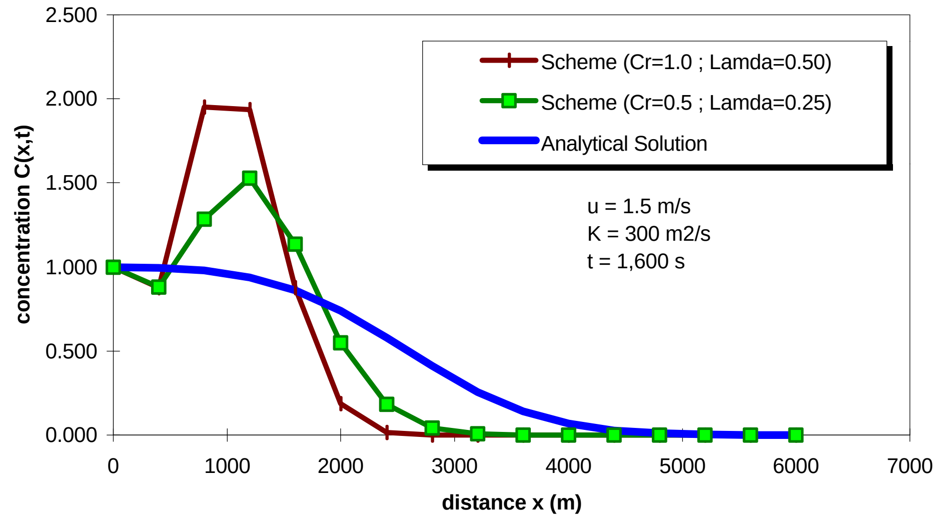

Figure 1. Oscillatory behavior and overshooting of the scheme (Forward-differences), using the combined stability criteria.

With the idea of still using the explicit schemes to solve equation (2), we search for a stability criterion for the complete scheme (3), using the "ordinary differential equation analogy method", Aldama, 1985. Replacing the rounding errors in the scheme (3), we can write:

$$R_i^{n+1} = A_0 R_{i-1}^n + A_1 R_i^n + A_2 R_{i+1}^n \qquad (4)$$

and by Fourier series we obtain the following equation:

$$\zeta = A_0 e^{-i\beta} + A_2 e^{i\beta} + A_1 \qquad (5)$$

Substituting the coefficients of central differences in space from table 1, equation (5) is transformed into:

$$\zeta = 1 + 2\lambda(\cos\beta - 1) - iCr\sin\beta \qquad (6)$$

now factoring Cr and replacing lamda=Cr/Pe in equation (6) yields to:

$$\zeta = 1 + Cr\left[\frac{2(\cos\beta - 1)}{Pe} - i\sin\beta\right] \qquad (7)$$

It is convenient to write equation (7) as:

$$\zeta = 1 + \mu \qquad (8)$$

where

$$\mu = Cr\left[\frac{2(\cos\theta - 1)}{Pe} - i\sin\theta\right] \qquad (9)$$

Accordingly to the Aldama method, let us consider the equation:

$$\frac{dy}{dt} = \delta y \qquad (10)$$

where y is an arbitrary time-dependent variable; delta, a complex coefficient; and t, time. The forward approximation to equation (10) is:

$$\frac{y_{n+1} - y_n}{\Delta t} = \delta y_n \qquad (11)$$

Solutions to the difference equation (10) are of the form (Gear, 1971):

$$y_n = \zeta^n \qquad (12)$$

and introducing equation (12) in (11), we get:

$$\zeta = \mu_0 + 1 \qquad (13)$$

where

$$\mu_0 = \delta \Delta t \qquad (14)$$

Expression (13) is exactly of the same form as equation (8), this means that the stability properties of schemes (3) and (11) are similar. Values on the boundary (where the Cauchy condition is satisfied), are of the form:

$$\zeta = e^{i\theta} - 1 \quad ; \quad 0 \le \theta \le 2\pi \qquad (15)$$

Thus, substituting (15) in (13) we can solve for the values of μ that define the stability boundary in the complex plane:

$$\mu_0 = e^{i\theta} - 1 \qquad (16)$$

The values of μ as defined by (9), for which scheme (3) is neutrally stable, have to satisfy the condition

$$\mu = |\mu_0| e^{i\phi_0} \qquad (17)$$

where phi represents an angular argument in the complex plane.

From equations (9) and (17) we get the following relations:

$$|\lambda_0| = Cr\left[\frac{4(\cos\beta - 1)^2}{Pe^2} + \sin^2\beta\right]^{1/2} \qquad (18)$$

$$\phi_0 = \tan^{-1}\frac{Pe\sin\beta}{2(\cos\beta - 1)} \qquad (19)$$

We are interested to obtain, for a given Péclét number, the smallest value of the corresponding Courant number. This means to solve the optimization problem:

$$Cr = \min_{\beta} \frac{|\lambda_0|}{\left[\frac{4(\cos\beta - 1)^2}{Pe^2} + \sin^2\beta\right]^{1/2}} \qquad (20)$$

subject to restrictions (17) and (19). The optimization problem was solved numerically and the result is presented in the form of the stability curve shown in figure 2. It can be noted there that for the range of small grid Péclét numbers (Pe<2), that the curve has a slope described by Cr< Pe/2.

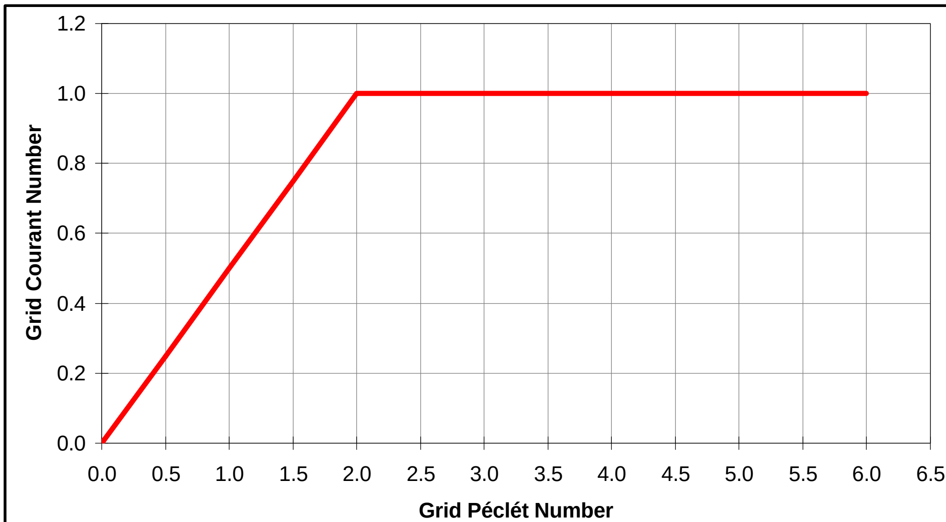

Figure 2. Stability curve. Critical Courant Number as a function of the Grid Péclét Number

Similar analysis were performed for the forward and backward difference approximations in space, and the results are summarize in table 2.

Table 2. *Results of Stability Conditions for Schemes*

Cr limit	Scheme	G value	Pe limit
$Cr = \frac{Pe}{2+G\,Pe}$	Backward	+ 1	Pe > 0
	Central	0	Pe < 2
	Forward	- 1	Pe < 1

Comparing solutions

The one-dimensional semi-infinite diffusion-advection problem seems to have become the standard test for determining the suitability of a numerical scheme design to solve the dispersion equation. For a continuous discharge of pollutant, the initial and boundary conditions are given by: C(x,0) = 0 and C(0,t) = Co. The solution to this problem is in Fischer, 1967. Results of applying the stability criterion found here are tested for the scheme (3) with central-difference approximations. The results are presented in figure 3.

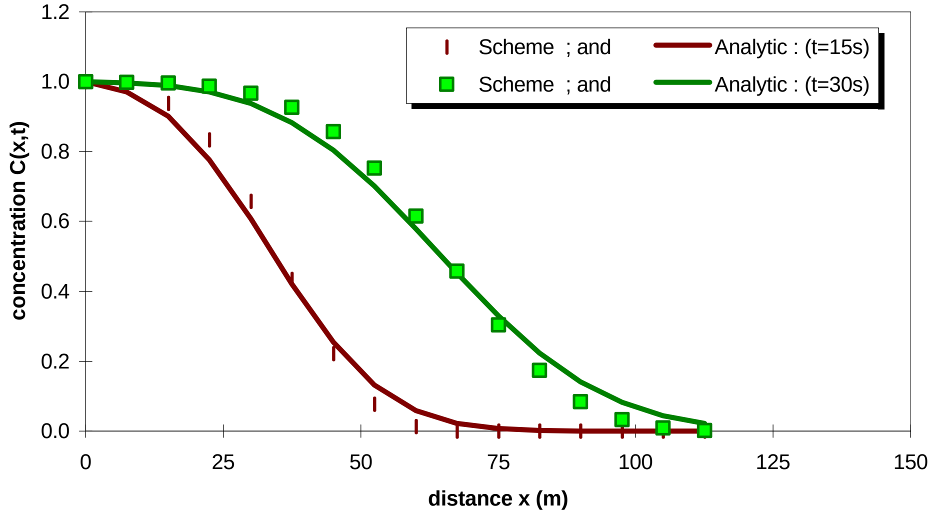

Figure 3. Comparison of results. Analytical vs. Central Scheme

Conclusions

A new stability analysis for the full advection-diffusion equation in its one-dimensional form is presented, giving the criterion of stability as a function of both local Courant and Péclét numbers. This relation restricts by itself, the values of the increments of time and space. Results obtained with the criterion found in this paper are very satisfactory.

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