

# Stability of the Standard Crank-Nicolson-Galerkin Scheme Applied to the Diffusion-Convection Equation: Some New Insights

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A stability analysis of the classical Crank-Nicolson-Galerkin (CNG) scheme applied to the one-dimensional solute transport equation is proposed on the basis of two fairly different approaches. Using a space-time eigenvalue analysis, it is shown, at least for subsurface hydrology applications, that the CNG scheme is theoretically stable under the condition  $PeCr \leq 2$ , where  $Pe$  and  $Cr$  are the mesh Péclet and Courant numbers. Then, to assess the computational stability of the scheme, the amplification matrix is constructed, and its norm is displayed in the  $(Pe, Cr)$  space. The results indicate that the norm of the amplification matrix is never smaller than unity and exhibits a hyperbolic nature analogous to the above theoretical condition.

## INTRODUCTION

Due to the importance of the space-time domain investigated in practical subsurface flow simulations, the association of finite element and finite difference techniques often leads to coarse discretizations. In such conditions the treatment of the diffusion-convection equation generally gives rise to high mesh Péclet ( $Pe$ ) and/or Courant ( $Cr$ ) numbers (convective dominance). In this type of problem, the wiggly and unstable behavior of standard schemes is well known [e.g., Gray and Pinder, 1976; Leonard, 1979; Gresho and Lee, 1979; Daus et al., 1985], and its corrupting effects prevent numerical convergence toward reasonable results.

In a fully convective problem (i.e.,  $Pe = \infty$ ) it was demonstrated in a previous paper [Noorishad et al., 1992] that more sophisticated nondiffusive finite elements methods [e.g., Brooks and Hughes, 1982; Donea et al., 1987; Westerink and Shea, 1989] have some difficulties when the transport of sharp fronts has to be simulated. To perform efficiently these Petrov- or Taylor-Galerkin methods requires a careful determination of  $Pe$  and  $Cr$  numbers as well as a relatively flexible set of initial conditions. However, in most three-dimensional practical problems, finite elements are coarse and irregular. In these cases a rigorous check of  $Pe$  and  $Cr$  is no longer possible, or nonunique, and initial solute fronts are often sharp.

For operational purposes, Noorishad et al. [1992] suggest to introduce in the commonly used Crank-Nicolson-Galerkin (CNG) scheme a very simple corrective function with the help of the dispersion tensor. This corrective function can be interpreted as an extra longitudinal dispersion which acts only at the points and in the directions that require to be stabilized. This approach was inspired by the early remedies developed for steady state convection-dominated transport [e.g., Hughes and Brooks, 1979; Kelly et al., 1980], and the extension to transient situations was based on an empirical stability criterion. The latter was derived from the second-order truncation error in the Taylor series expansion of the transient term in the transport equation. As was suggested by Noorishad et al. [1992], the respect of the condition

$PeCr \leq \gamma$ , with  $\gamma$  as a performance index ( $2 \leq \gamma \leq 10$ ), along the flow lines is suitable for solving practical linear problems. Results are stable and do not show overdiffusion signals. This simple technique leads to robust algorithms which are directly applicable to more complicated problems such as convective coupled transfers involving sharp fronts [Perrochet and Kiraly, 1991].

It is important to recall that when the standard CNG scheme is applied to the diffusion-convection equation, there is a limit in the solution domain that defines two regions in which transport is dominated by either diffusion or convection. In this latter region nonphysical oscillations generally affect the numerical solutions. This limit is generally defined by means of the  $Pe$  and  $Cr$  numbers. When both conditions  $Pe \leq 2$  and  $Cr \leq 1$  are fulfilled the CNG scheme is stable (no oscillations). The above two conditions have been established according to theoretical considerations [Price et al., 1966; Daus et al., 1985], and it is frequently recommended in the specialized literature that they should be systematically respected. On the basis of numerical experiments, Huyakorn and Pinder [1983, p. 206] indicate that the criterion  $Pe \leq 10$  is still suitable if mild residual oscillations can be accepted. It has to be noted here that this experimental result corresponds also to the maximum value of the performance index  $\gamma$  in the CNG scheme when  $Cr$  approaches unity.

The present paper provides additional theoretical information to the one of Noorishad et al. [1992], which was more concerned with the comparative assessment of contemporary finite element numerical schemes. The empirical stability criterion  $PeCr \leq 2$  is confirmed here by a revised eigenvalue analysis performed on the CNG matrix equations. Moreover, to complete this theoretical analysis, the amplification of numerical errors due to time stepping is evaluated by means of a norm analysis of the CNG amplification matrix throughout the  $(Pe, Cr)$  space.

## BASIC EQUATIONS

In the context of a one-dimensional, nonreactive solute transport in a homogeneous porous saturated media without sources, the diffusion-convection equation may be written as

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

where  $C = C(x, t)$  is the solute relative concentration (dimensionless),  $v$  is the average pore velocity (meters per second), and  $D$  is the dispersion coefficient (square meters per second) normally defined as

$$D = \alpha_L v + D_m \quad (2)$$

with  $\alpha_L$  being the longitudinal dispersivity (meters) and  $D_m$  the molecular diffusion coefficient (square meters per second).

When the space-time domain  $(x, t)$  is discretized, the size of the elementary grid defined by  $\Delta x$  and  $\Delta t$  characterizes the simulation by means of the adimensional  $Pe$  and  $Cr$  numbers.  $Pe$  is the ratio between the length of the elementary trajectory and the total mixing length  $\alpha_L + D_m/v$  along the flow direction, and  $Cr$  is the ratio between the convective distance covered by a water particle during the time step  $\Delta t$  and the space increment  $\Delta x$ . In the one-dimensional case these two-adimensional numbers are simply

$$Pe = v\Delta x/D \quad Cr = v\Delta t/\Delta x \quad (3)$$

The above equations show that it is very difficult to meet simultaneously the classical constraints (i.e.,  $Pe \leq 2$  and  $Cr \leq 1$ ) when simulating low diffusive transport problems. For high-flow velocities and/or low diffusion-dispersion effects,  $\Delta x$  has to be reduced to keep  $Pe \leq 2$ . With such a high space resolution, reducing the time step to very low values is then the only way to satisfy the constraint  $Cr \leq 1$ . Such a detailed space-time discretization is probably acceptable when simulating one-dimensional transfers in laboratory columns or small volumes. This is no longer the case in real practical problems which have to be analyzed on a two- or even three-dimensional basis and involve large volumes. As a matter of fact, the length of the elementary trajectory can only be calculated with good accuracy if the problem remains one dimensional. Moreover, this length can not be determined precisely in very heterogeneous media. It can hardly be estimated in unsteady flow conditions and/or when the shape of the finite elements is irregular. Since most practical problems involve a combination of these different features, the only way out is to achieve an extremely detailed space-time resolution which in most cases requires sophisticated hardware equipment not always available or profitable.

In the context of field studies, the analysis presented below demonstrates the relevance of a very practical stability criterion which considerably widens the operational solution domain of the standard CNG scheme.

#### EIGENVALUE ANALYSIS OF THE CNG SCHEME

Using the basic concepts relative to Liapounov's stability theory [e.g., *Piskounov*, 1976, pp. 127–137], this eigenvalue analysis is based on a "two-step" treatment of the transport equation. In the first place, the effect of the finite element discretization (Galerkin) on the time behavior of the general solutions is evaluated. Second, the impact of discretizing time with central finite differences (Crank-Nicolson) on the spatial behavior of the general solutions is assessed.

Considering the one-dimensional diffusion-convection equation (1) and applying a space discretization to the right-hand side terms, one obtains for a linear element and after integration the typical divergence element matrix

$$\mathbf{A}^e = \begin{bmatrix} \frac{D}{\Delta x} + \frac{v}{2} & -\frac{D}{\Delta x} + \frac{v}{2} \\ \frac{D}{\Delta x} - \frac{v}{2} & \frac{D}{\Delta x} - \frac{v}{2} \end{bmatrix} \quad (4)$$

Assembling this element matrix for a network with  $p$  linear elements and  $N = p + 1$  nodes leads to a global tridiagonal matrix  $\mathbf{A}_{N \times N}$ . Equation (1) can then be written under the semi-discrete form

$$\frac{\partial(C_i)}{\partial t} = - \begin{bmatrix} \frac{D}{\Delta x} + \frac{v}{2} & -\frac{D}{\Delta x} + \frac{v}{2} & 0 & \cdots & 0 \\ & & & & \vdots \\ -\frac{D}{\Delta x} - \frac{v}{2} & \frac{2D}{\Delta x} & \cdots & & 0 \\ 0 & \cdots & \frac{2D}{\Delta x} & -\frac{D}{\Delta x} + \frac{v}{2} \\ \vdots & & & & \\ 0 \cdots & 0 & -\frac{D}{\Delta x} - \frac{v}{2} & \frac{D}{\Delta x} - \frac{v}{2} \end{bmatrix} (C_i) \quad (5)$$

where  $C_i$  represents the concentration at a given point with coordinate  $x_i$ . The behavior of the general solutions  $C(x_i, t)$  depends on the eigenvalues of the coefficient matrix  $\mathbf{A}$ . If the number of nodes  $N$  is high enough ( $N > 15$  according to *Daus et al.* [1985]), the tridiagonal coefficient matrix may be assimilated to a Toeplitz matrix (a single value in each diagonal) for which eigenvalues are

$$\lambda_k = -\frac{2D}{\Delta x} + 2 \left( \frac{D^2}{\Delta x^2} - \frac{v^2}{4} \right)^{1/2} \cos \left( \frac{\pi k}{N+1} \right) \quad (6)$$

$$k = 1, 2, \dots, N$$

Equation (6) shows that the eigenvalues of (5) become complex when  $D/\Delta x < v/2$  (i.e.,  $Pe > 2$ ) and that they always present negative real parts (i.e.,  $\text{Re}(\lambda_k) < 0$ ). In this case, according to Liapounov's stability theory, the general solutions are of a damped oscillatory nature. Small disturbances at points with coordinates  $x_i$  propagate in time according to periodic damped functions, and it can be thus concluded that the general unknown functions  $C(x_i, t)$  are unconditionally stable. Similar results are obtained with the von Neumann stability analysis [i.e., *Pinder and Gray*, 1977, pp. 150–169].

Since the CNG scheme generates highly unstable and oscillatory results in cases where convection dominates, it seems obvious that the stability of the CNG method is not unconditional, as stated above, but depends on a criterion which can not be directly derived from the analysis of system (5).

Instead of concentrating on the analysis of the temporal stability of the function  $C(x_i, t)$ , as most researchers do, it is also important to assess the spatial stability of functions  $C(x, t^n)$  (see Figure 1). This procedure is entirely justified since in most applications both space and time stabilities have to be guaranteed. Moreover, in the context of practical problems, engineers are specially interested in obtaining stable concentration profiles at given times.

To apply the Liapounov principles to a space stability

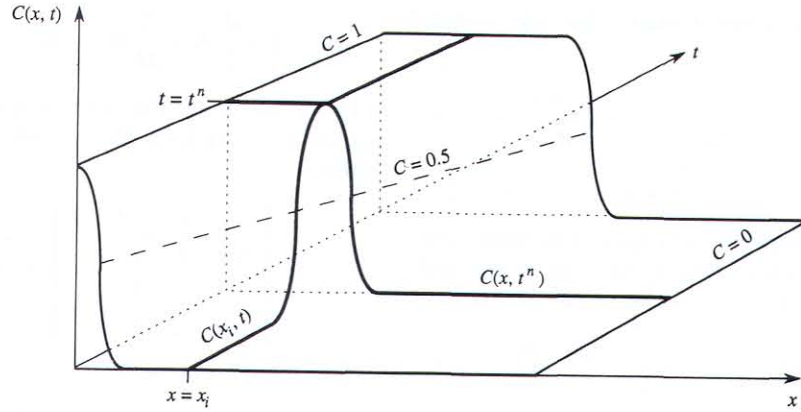


Fig. 1. Continuous one-dimensional injection case. Schematic view of space-time function  $C(x, t)$  with "sections"  $C(x_i, t)$  and  $C(x, t^n)$ .

analysis, it is necessary to write a system of equations which is similar to that in (5), but this time with first space derivatives  $\partial C^n / \partial x$  in the left-hand side and only time terms in the right-hand side. Since the form of (1) is not readily suitable for such an operation, the following transformation is proposed.

Taking the partial derivative of the reference equation (1) with respect to time and reversing the derivation indexes gives

$$C_{tt} = -v \partial_t C_x + D \partial_t C_{xx} = -v \partial_x C_t + D \partial_{xx} C_t \quad (7)$$

Substituting in this equation the first time derivative  $C_t$  by its expression in the basic equation (1) yields

$$C_{tt} = v^2 C_{xx} - 2vDC_{xxx} + D^2 C_{xxxx} \quad (8)$$

which can be written as

$$C_{xx} = \frac{1}{v^2} C_{tt} + \frac{2D}{v} C_{xxx} - \frac{D^2}{v^2} C_{xxxx} \quad (9)$$

If (9) is now substituted into (1), one obtains an alternative form for the transport equation which reads after rearranging terms

$$C_x = -\frac{1}{v} C_t + \frac{D}{v^3} C_{tt} + \frac{2D^2}{v^2} C_{xxx} - \frac{D^3}{v^3} C_{xxxx} \quad (10)$$

Considering standard values commonly used in groundwater hydrology for  $v$  and  $D$  (for instance,  $v = 10^{-5}$  m/s and  $D = 10^{-7}$  m<sup>2</sup>/s) it can be seen that coefficients multiplying the third- and fourth-order space derivatives ( $2 \times 10^{-4}$  and  $10^{-6}$ ) are negligible compared to those that multiply the first and second time derivatives ( $10^5$  and  $10^8$ ). Consequently, (10) is left with

$$\frac{\partial C}{\partial x} = -\frac{1}{v} \frac{\partial C}{\partial t} + \frac{D}{v^3} \frac{\partial^2 C}{\partial t^2} \quad (11)$$

which is the form required to perform the space stability analysis of the solution  $C(x, t^n)$ . Applying the central Crank-Nicolson treatment to the right-hand side terms of (11), one obtains the typical difference equation at time level  $t^n$

$$\frac{\partial C^n}{\partial x} = -\frac{1}{v} \left( \frac{C^{n+1} - C^{n-1}}{2\Delta t} \right) + \frac{D}{v^3} \left( \frac{C^{n+1} - 2C^n + C^{n-1}}{\Delta t^2} \right) \quad (12)$$

For a sufficient number  $M$  of temporal levels, (11) may now be expressed under the semidiscrete form

$$\frac{\partial(C^n)}{\partial x} = - \begin{bmatrix} \frac{2D}{v^3 \Delta t^2} & -\frac{D}{v^3 \Delta t^2} + \frac{1}{2v \Delta t} & 0 & \cdots & 0 \\ \frac{D}{v^3 \Delta t^2} - \frac{1}{2v \Delta t} & \frac{2D}{v^3 \Delta t^2} & \ddots & & \\ 0 & \ddots & \frac{2D}{v^3 \Delta t^2} & -\frac{D}{v^3 \Delta t^2} + \frac{1}{2v \Delta t} & \\ \vdots & & & & \\ 0 & \cdots & 0 & -\frac{D}{v^3 \Delta t^2} - \frac{1}{2v \Delta t} & \frac{2D}{v^3 \Delta t^2} \end{bmatrix} (C^n) \quad (13)$$

in which the tridiagonal Toeplitz matrix has eigenvalues given by

$$\lambda_k = -\frac{2D}{v^3\Delta t^2} + 2\left(\frac{D^2}{v^6\Delta t^4} - \frac{1}{4v^2\Delta t^2}\right)^{1/2} \cos\left(\frac{\pi k}{M-1}\right) \quad (14)$$

$$k = 1, 2, \dots, M-2$$

In this case, if the solutions  $C(x, t^n)$  have to be stable and nonoscillatory space functions, the  $\lambda_k$  have to be real and negative numbers. Therefore the condition for stability is

$$\frac{D^2}{v^6\Delta t^4} \geq \frac{1}{4v^2\Delta t^2} \quad 4 \geq \frac{v^4\Delta t^2}{D^2} \quad 2 \geq \frac{v\Delta x}{D} \frac{v\Delta t}{\Delta x} \quad (15)$$

or, using the definitions (3),

$$PeCr \leq 2 \quad (16)$$

Within the validity limits of the simplifications inherent in (10), a limiting constraint that preserves the stability of the CNG scheme has been established from robust theoretical considerations. One should note that unlike the classical analysis of Taylor expansions up to an arbitrary given order, the truncation of (10) from the third order is physically justified here, at least for subsurface hydrology applications.

#### ERROR AMPLIFICATION OF THE CNG SCHEME

In this section, the norm of the CNG amplification matrix is analyzed to evaluate the propagation and amplification of the various errors arising from the discretization scheme during time stepping. Surprisingly, this procedure, which has been applied several times in the past for diffusion type problems [e.g., *Huyakorn and Pinder*, 1983, pp. 59–62], has not been so widely reported in the context of diffusion-convection equations. This last point might be explained by the fact that the outcome of such an analysis is somewhat in contradiction with the common notion of numerical stability. The latter requiring the nonamplification (dampening) of numerical errors through time.

Following *Huyakorn and Pinder* [1983], a time stepping scheme can be expressed in the general matrix form

$$\mathbf{L}\mathbf{C}^{t+\Delta t} = \mathbf{R}\mathbf{C}^t \quad (17)$$

where  $\mathbf{C}^{t+\Delta t}$  and  $\mathbf{C}^t$  are the unknown and initial solution vectors for the current time step, respectively, and  $\mathbf{L}$  and  $\mathbf{R}$  are for the Crank-Nicolson procedure

$$\mathbf{L} = \frac{1}{2}\mathbf{A} + \frac{1}{\Delta t}\mathbf{B} \quad \mathbf{R} = -\frac{1}{2}\mathbf{A} + \frac{1}{\Delta t}\mathbf{B} \quad (18)$$

In (18)  $\mathbf{A}$  and  $\mathbf{B}$  are the global divergence and capacitance matrices resulting from the assembly of the Galerkin element matrices

$$\mathbf{A}^e = \begin{bmatrix} \frac{D}{\Delta x} + \frac{v}{2} & -\frac{D}{\Delta x} + \frac{v}{2} \\ -\frac{D}{\Delta x} - \frac{v}{2} & \frac{D}{\Delta x} - \frac{v}{2} \end{bmatrix} \quad \mathbf{B}^e = \begin{bmatrix} \Delta x & \Delta x \\ 3 & 6 \\ \Delta x & \Delta x \\ 6 & 3 \end{bmatrix} \quad (19)$$

Equation (17) can be written

$$\mathbf{C}^{t+\Delta t} = \mathbf{G}\mathbf{C}^t \quad (20)$$

in which  $\mathbf{G} = \mathbf{L}^{-1}\mathbf{R}$  is referred to as the amplification matrix. The error vector at time level  $t$  is defined as

$$\mathbf{E}^t = \hat{\mathbf{C}}^t - \mathbf{C}^t \quad (21)$$

where  $\hat{\mathbf{C}}^t$  denotes the exact solution at time level  $t$ . Since (20) is also satisfied by  $\hat{\mathbf{C}}^t$  and  $\hat{\mathbf{C}}^{t+\Delta t}$ , it follows by subtraction that

$$\mathbf{E}^{t+\Delta t} = \mathbf{G}\mathbf{E}^t \quad (22)$$

or, after  $m$  time steps,

$$\mathbf{E}^{t+m\Delta t} = \mathbf{G}^m\mathbf{E}^t \quad (23)$$

Taking compatible matrix and vector norms (here the norm  $\|\cdot\|_2$  is enforced) and making use of the Schwartz inequalities, one obtains

$$\|\mathbf{E}^{t+m\Delta t}\| = \|\mathbf{G}^m\mathbf{E}^t\| \leq \|\mathbf{G}\|^m\|\mathbf{E}^t\| \quad (24)$$

and it is apparent that the error will not grow with time if

$$\|\mathbf{G}\| \leq 1 \quad (25)$$

The spectral norm of a nonsymmetric matrix like  $\mathbf{G}$  can be calculated by [e.g., *Ciarlet*, 1982]

$$\|\mathbf{G}\| = \sup \frac{\|\mathbf{G}\mathbf{E}\|}{\|\mathbf{E}\|} = \left( \max_k (\lambda_k(\mathbf{G}^T\mathbf{G})) \right)^{1/2} \quad (26)$$

where  $\lambda_k$  is the eigenvalue spectrum of  $\mathbf{G}^T\mathbf{G}$ , which maximum is the square of the greatest singular value of  $\mathbf{G}$  (i.e., the norm of  $\mathbf{G}$ ).

$$\mathbf{L} = \begin{bmatrix} \frac{Cr}{2Pe} + \frac{Cr}{4} + \frac{1}{3} & -\frac{Cr}{2Pe} + \frac{Cr}{4} + \frac{1}{6} & 0 & \dots & 0 \\ \frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{6} & \frac{Cr}{Pe} + \frac{2}{3} & \dots & \dots & 0 \\ 0 & \dots & \frac{Cr}{Pe} + \frac{2}{3} & -\frac{Cr}{2Pe} + \frac{Cr}{4} + \frac{1}{6} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & -\frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{6} & \frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{3} \end{bmatrix} \quad (27a)$$

$$\mathbf{R} = \begin{bmatrix} \frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{3} & \frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{6} & 0 & \dots & 0 \\ \frac{Cr}{2Pe} + \frac{Cr}{4} + \frac{1}{6} & -\frac{Cr}{Pe} + \frac{2}{3} & \dots & \dots & 0 \\ 0 & \dots & -\frac{Cr}{Pe} + \frac{2}{3} & \dots & \frac{Cr}{2Pe} - \frac{Cr}{4} + \frac{1}{6} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & \dots & 0 \end{bmatrix} \quad (27b)$$

Assembling element matrices  $\mathbf{A}^e$  and  $\mathbf{B}^e$  for  $p$  linear elements ( $N = p + 1$  nodes) and constructing the  $N \times N$  matrices  $\mathbf{L}$  and  $\mathbf{R}$  in an adimensional form yields

From these two global matrices it is seen that the amplification matrix is entirely defined by the numbers  $Pe$  and  $Cr$  characterizing the simulation. Hence using (26), the function  $\|\mathbf{G}(Pe, Cr)\|$  can be computed and analyzed throughout the  $(Pe, Cr)$  space. It has to be noted here that the variations of  $\|\mathbf{G}\|$  with an increasing number  $p$  of elements stop to be significant for  $p > 10$ . The function  $\|\mathbf{G}(Pe, Cr)\|$  is illustrated for  $p = 20$  on Figure 2(top) with contours  $\Delta\|\mathbf{G}\| = 0.2$ . Contours greater than 2 are not shown to preserve picture clarity.

A first important remark concerning Figure 2(top) is that  $\|\mathbf{G}\|$  is always greater than unity as long as the convective velocity  $v$  is not zero, and even for very fine time and/or space increments. It is also visible on Figure 2(bottom) that the hyperbolic shape of the function  $\|\mathbf{G}\| = 2$  is very similar to the stability limit  $PeCr = 2$  resulting from the eigenvalue analysis. Hence and even for the classical simultaneous constraints  $Pe \leq 2$  and  $Cr \leq 1$ , the condition (25) controlling the dampening of residual numerical errors during time stepping is never satisfied. From a theoretical point of view, this last statement implies a risk to see the numerical solution becoming highly unstable (errors propagating and increasing without bounds) for simulations involving many time steps. However, nevertheless, practical experience has shown that the CNG scheme could be safely used for a large variety of diffusion-convection problems.

This apparent contradiction may be explained by the fact that although  $\|\mathbf{G}\| > 1$  in (24),  $\|\mathbf{E}^{t+m\Delta t}\|$  can still remain reasonable if the initial error  $\|\mathbf{E}^t\|$  is very small (i.e., round-off errors). The important inequality  $\|\mathbf{G}^m\| \ll \|\mathbf{G}\|^m$  ( $m \gg 1$ ) also shows that error amplification at each time step is actually far less than  $\|\mathbf{G}\|$ . Moreover, it was checked for a wide range of  $Pe$  and  $Cr$  values that the ratio  $\|\mathbf{G}^{m+1}\|/\|\mathbf{G}^m\|$  was rapidly converging toward unity after a few tens of time steps.

For the purpose of information, it can be noted at this point that the above amplification analysis has also been applied to other contemporary finite element schemes [Perrochet, 1993]. Higher-order methods designed for solving highly convective transport problems, namely, the schemes Streamline-Upwind-Petrov-Galerkin (SUPG) [Brooks and Hughes, 1982], Crank-Nicolson-Taylor-Galerkin (CNTG), [Donea et al., 1987] and Streamline-Upwind-Full-Galerkin (SUFG) [Perrochet, 1993], were investigated and compared

to standard methods in terms of accuracy and stabilizing properties. Since all these schemes turned out to show amplification factors always greater than unity, one may think that the criterion (25) is not appropriate for defining the

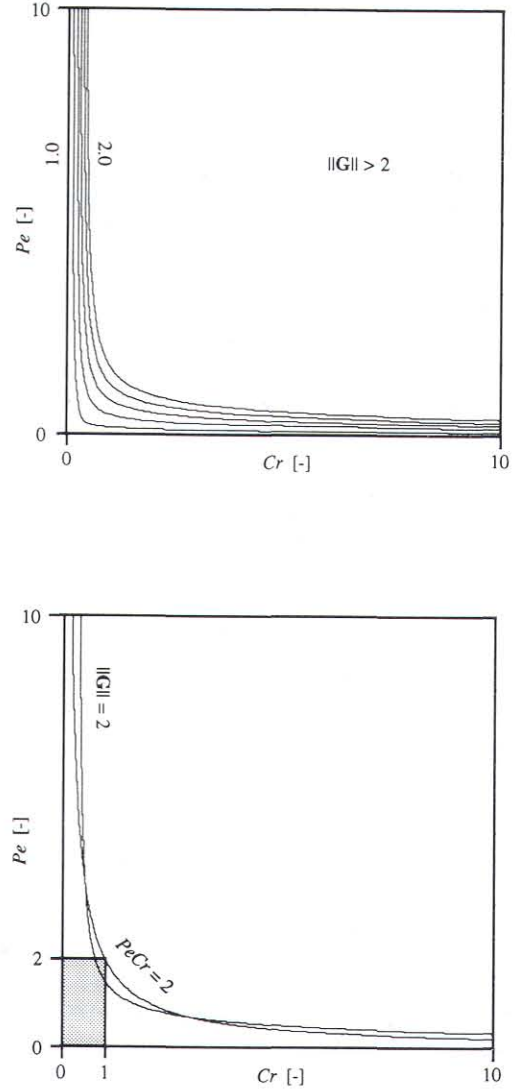


Fig. 2. Norm of the amplification matrix and stability domain for the CNG scheme. (Top) Contours of the function  $\|\mathbf{G}(Pe, Cr)\|$  and (bottom) stability limit  $PeCr = 2$  with classical constraints  $Pe \leq 2$  and  $Cr \leq 1$ , and with function  $\|\mathbf{G}(Pe, Cr) = 2$ .

stability limits of diffusion-convection algorithms. However, the function  $\|G\|$ , indeed, remains an excellent indicator to assess the relative sensitivity and robustness of various schemes toward space-time discretization.

#### FINAL REMARKS

The stability condition  $PeCr \leq 2$  introduced on an empirical basis in the work by *Noorishad et al.* [1992], and for which the conventional constraints ( $Pe \leq 2$  and  $Cr \leq 1$ ) are only a particular case, has been theoretically confirmed here. This new criterion indicates that convection dominated transport problems (i.e., high  $Pe$  number) can be safely simulated with the standard CNG method provided  $Cr$  is consequently reduced. Compared to the conventional constraints, and apart from an important extension of the stability domain, a major characteristic of this criterion is that it can be readily expressed in a very practical operational form. Moreover, its nature directly leads to the most reasonable way to achieve transient ‘‘smart upwinding’’ if the latter is needed.

Adopting the multidimensional definition of  $Pe$  and  $Cr$  [e.g., *Yu and Heinrich*, 1987] and prescribing the respect of the condition  $PeCr \leq 2$  along the flow lines, one obtains

$$\frac{\|\mathbf{v}\|^2 \Delta t}{\|\mathbf{v}\|(\alpha_L + D_m/\|\mathbf{v}\|)} \leq 2 \quad (28)$$

and it is obvious that the above inequality can be satisfied, without requiring the determination of  $Pe$  and  $Cr$  numbers, if

$$\alpha_L \geq \frac{\|\mathbf{v}\| \Delta t}{2} - \frac{D_m}{\|\mathbf{v}\|} \quad (29)$$

For a given time step  $\Delta t$ , (29) clearly indicates that a stable solution is obtained if the total mixing length is at least equal to half of the convective distance  $\|\mathbf{v}\| \Delta t$ . In regions of the model domain where the physical longitudinal dispersivity  $\alpha_L$  is not enough, an additional longitudinal dispersivity  $\overline{\alpha}_L$  can be added up to the minimum required following the rule

$$\overline{\alpha}_L = \frac{\|\mathbf{v}\| \Delta t}{2} - \alpha_L - \frac{D_m}{\|\mathbf{v}\|} \quad \text{with} \quad \overline{\alpha}_L = 0 \quad (30)$$

$$\text{if} \quad \alpha_L + \frac{D_m}{\|\mathbf{v}\|} \geq \frac{\|\mathbf{v}\| \Delta t}{2}$$

In addition, when small residual oscillations can be tolerated in the solution, the factor 2 in (28)–(30) can be replaced by the performance index  $\gamma$  mentioned in the introduction. One should note here that the relevance of this parameter is reinforced by the shape of the amplification curves in Figure 2(top).

When analyzing field problems at a regional scale, condition (30) has significant advantages with respect to traditional diffusive schemes such as Implicit-Galerkin (IMG) and Upwind-Crank-Nicolson-Galerkin (UCNG) [*Huyakorn and Nilkuha*, 1979], particularly in the case of multidimensional modeling. Unlike the IMG scheme in which every point in the flow domain is subjected to the implicit treatment and the related excessive smearing, the fulfillment of condition (30) by the CNG scheme precisely limits to a strict minimum the quantity of artificial diffusion needed for stability. In other

words, the latter only acts (differentially) at integration points and along directions for which a corrective action is required. For this reason, it can be stated that the proposed criterion brings the performances of the CNG scheme to an optimum level.

With respect to the techniques of the UCNG type, the CNG scheme associated with condition (30) requires neither the definition of asymmetric weighting functions nor the calculation of upwind parameters which in most practical cases is not very easy. Moreover, since the asymmetric weighting functions can only generate a limited quantity of stabilizing diffusion, approaches of the UCNG type are no longer effective when local values of the Courant number exceed one.

The above considerations have been tested and checked by means of numerical experiments and comparative test problems relative to linear and nonlinear transport [*Noorishad et al.*, 1992; *Perrochet and Kiraly*, 1991]. Some large-scale applications [*Perrochet*, 1992] have also proven the efficiency of the proposed method.

Finally, it may not be useless to remind potential users that the apparently good solutions provided by this method are not likely to be the exact solutions to given problems, but rather the best approximations that a standard technique can achieve given a real world discretization.

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