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The one-dimensional transient diffusional method: finite element adaptive solutions to convection–diffusion problems

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Abstract — The diffusional method, a new, simple and natural concept, is introduced for solving convection–diffusion equations. The inherent formulation leads to the variational scheme for one-dimensional steady-state problems; however, the formulation is general and can be directly used in multidimensional analysis. Additionally, a lumped capacitance (mass) matrix first-order time integration technique is presented that is unconditionally stable in its implicit form and conditionally stable for Courant numbers less than one in its explicit form. The explicit form is shown, by comparison with a two-step Taylor–Galerkin scheme, to present an excellent performance for solving transient boundary layer problems and Burger's non-linear equation. Because of dampening due to first order accuracy of the time integrator, the method is not well suited to solve advection dominated problems involving travelling waves at high Péclet numbers; in this respect, a brief analysis is made on the explicit form of the Taylor–Galerkin scheme. This work also presents a performance analysis of the method when used in conjunction with adaptive time stepping procedures. The resulting adaptive PMGV scheme works very well for boundary layer problems and for solving Burger's non-linear viscous and non-viscous equations. © 1999 Éditions scientifiques et médicales Elsevier SAS.

convection-diffusion / finite elements / variational method / Petrov-Galerkin method / diffusional method

Résumé — **Méthode de diffusion transitoire unidimensionnelle : solutions adaptatives par la méthode des éléments finis appliquée aux problèmes de convection–diffusion.** La méthode de diffusion, un concept nouveau, simple et naturel, est présentée pour résoudre des équations de convection–diffusion. La formulation inhérente mène au schéma variationnel pour des problèmes unidimensionnels en régime stationnaire ; cependant la formulation est générale et peut être utilisée directement dans l'analyse multidimensionnelle. En outre, on présente une technique d'intégration temporelle de premier ordre utilisant une forme concentrée de la matrice de capacitance. Cette technique est inconditionnellement stable dans ses formes implicites et conditionnellement stable pour des nombres de Courant plus petits que l'unité dans sa forme explicite. Par comparaison avec le schéma Taylor–Galerkin de deux pas, la forme explicite présente une performance excellente pour résoudre des problèmes de couche limite transitoire et l'équation non linéaire de Burger. La méthode n'est pas tout à fait convenable, à cause de l'amortissement dû à l'exactitude de premier ordre de l'intégration temporelle, pour résoudre des problèmes dominés par l'advection en ce qui concerne des ondes voyageuses (*travelling waves*) à nombres de Péclet élevés ; sur ce sujet, on présente une petite analyse du schéma explicite de Taylor–Galerkin. On présente aussi une analyse de performance de la méthode diffusionnelle couplée à des procédés adaptatifs d'avancement temporel. Le schéma adaptatif PMGV résultant s'est montré particulièrement performant pour des problèmes de couche limite et pour la résolution des équations non linéaires de Burger. © 1999 Éditions scientifiques et médicales Elsevier SAS.

convection-diffusion / éléments finis / méthode variationnelle / méthode de Petrov-Galerkin / méthode diffusionnelle

Nomenclature

A parameter defined in equation (22)
A_m function defined in equation (57)
a_s coefficient defined in equation (8)
a_t coefficient defined in equation (15)
B parameter defined in equation (22)
B_m functions defined in equation (58)
b_s coefficient defined in equation (8)
b_t coefficient defined in equation (15)
C Courant number ($= u\,\Delta t/h$)

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$\boldsymbol{C}$ capacitance matrix
c_s coefficient defined in equation (8)
c_t coefficient defined in equation (15)
$\boldsymbol{D}$ force vector
d_i parameter defined in equation (8)
d^* parameter defined in equation (53)
F local Fourier number ($= G\,\Delta t/h^2$)
G amplification factor, defined in equation (41)
$\widehat{G}$ amplification factor, defined in equation (38)
G^* ratio of the amplification factors
h step size
$\boldsymbol{K}$ stiffness matrix
k wave number
ℓ wavelength
L characteristic length
n time level
N shape function
p parameter defined in equation (5)
P global Péclet number ($= u\,L/2\,\Gamma$)
Pe local Péclet number ($= u\,h/2\,\Gamma$)
Q source term
Re Reynolds number, dimensionless
t time
u x-velocity
v y-velocity
W weighting function
x spatial variable
y spatial variable

Greek symbols

α upwind parameter
β_m parameter defined in equation(59)
ϵ truncation error
λ argument defined in equation (39)
λ^* relative celerity
λ_m parameter defined in equation (59)
σ parameter defined in equation (46)
ϕ approximate value for the dependent variable
$\widehat{\phi}$ dependent variable
θ relaxation parameter
Γ diffusion coefficient

Superscripts

exact value
E exact solution
n time level
p predicted value

Subscripts

i space level
n time level
new new value
old old value
opt optimal value
s steady-state term
t transient term
x x direction
y y direction

1. INTRODUCTION

Since the seventies fast progress has been observed in the development of numerical and analytical techniques for solving convection-diffusion and fluid mechanics problems. Finite difference and finite volume methods [1–4] were, till the beginning of the eighties, the best established procedures. Today, due to the widespread use and improvements of early Petrov-Galerkin methods [5–6], such as the balancing diffusion scheme [7], the streamline upwind Petrov-Galerkin (SUPG) method [8], the consistent approximate upwind method [9-10] and other techniques, the finite element (FE) method has become extremely competitive with respect to the other numerical methods. However most of the FE proposed techniques present ad-hoc reasoning, and, although not leading to substantial errors, do not present optimal solutions to two or three-dimensional problems and thus require special manipulations for many kinds of problems. This work aims at contributing to the minimisation of the errors associated to these ad-hoc procedures.

The literature associated to FE solutions to convection-diffusion and fluid mechanics problems is copious and full reviews can be found elsewhere [11–15]. Steady-state one- dimensional Petrov–Galerkin and variational methods lead to optimal solutions. However, transient solutions arising from the variational method are generally unstable; those solutions arising from the Petrov–Galerkin formulation are unconditionally stable for implicit problems ($\theta \geq 0.5$) but show excessively dampened solutions; (Bubnov-) Galerkin's method has also been shown not to be appropriate for obtaining general transient or steady-state solutions [12]. One should notice that only heuristic arguments have been used to obtain two-dimensional formulations by the Petrov–Galerkin method.

Lagrangian methods, separately or combined with Eulerian methods, have been extensively used to solve transient advection-dominated problems. In this way, different particle tracking techniques, involving adaptive [16], adjustable hidden fine-mesh approach [17], modified single-step reverse particle tracking Eulerian-Lagrangian schemes [18] have been developed. However, these methods make use of either time consuming programming techniques or are not readily available for two- or multidimensional problems. Two- [19] and multidimensional [20–21] finite element methods of characteristics are available. A Taylor–Galerkin scheme originally proposed by Donea [22] and its one-dimensional equivalent characteristic-Galerkin formulation [11, 23]

were proven to perform better than the classical Lax-Wendroff and implicit Crank-Nicolson schemes [24–25]; their range of stability is limited to Courant numbers C, smaller than 0.57, unless a lumped mass matrix is used in an iterative procedure and, in this case, the stability limit increases to $C = 1$. A two-step Taylor–Galerkin formulation [24] has also been proved to work well; however the procedure is conditionally stable and the limiting C value is identical to the one related to the characteristic Galerkin method. The use of space-time elements [26–29], higher order methods [30–31] and $h - p$ finite element methods [13–14] for solving convection-diffusion problems are also available.

In addition, the literature associated to adaptive finite element mesh refinement techniques has grown considerably in the last decade [13,14,32-36]. Work has also been done on:

– steady-state adaptive finite element solutions to convection-diffusion and compressible and incompressible fluid mechanics problems [10, 37–39];

– transient mesh adaptive finite element [40–41] and finite-difference [42–43] schemes for diffusion problems;

– transient finite element schemes for advection-dominated or hyperbolic [16–18, 44] problems, convection-diffusion [45–46] problems and Navier–Stokes equations [47–48].

Solutions to transient convection–diffusion problems are problem-sensitive; thus, solving techniques applicable to travelling wave (advection-dominated) type problems may not be adequate for boundary layer problems; a scheme for linear problems may not work for non-linear problems [12]. Therefore, the basic algorithms used in mesh-adaptive/time-adaptive schemes when applied to convection-diffusion problems deserve more careful attention.

Of special interest to this work, Gresho et al [49] proposed an implicit adaptive time integrator based on a second-order accurate Adams–Bashforth predictor (ABP) and the trapezoid rule as the corrector. The ABP requires the evaluation of rates of change at previous time planes that are obtained through successive applications of the trapezoid rule. The corrector step uses again the trapezoid rule which is non-dissipative, completely stable and second-order accurate. Bixler [50] changed Gresho et al's integrator by incorporating three modifications: (1) the one leg-twin form of the trapezoid rule replaced the trapezoid rule as the corrector, leading to a more accurate local time truncation error estimate; (2) a more stable predictor was obtained by changing the expression for obtaining rates of change and (3) the formula used for predicting time-step size was redressed to match the new corrector. Bixler's scheme was used in adaptive procedures applied to heat transfer and the incompressible Navier–Stokes equations [47–48] and to thermal problems [45–46]. Gresho et al [49] also presented a scheme based upon Euler's forward (as predictor) and backward (as an implicit corrector) formulas; however, they suggested that the scheme should be used only for obtaining steady state solutions because of the dissipative nature of the resulting finite element (FE) scheme.

The specific objectives of this work are:

– to present a new and natural concept to solving convection-diffusion equations, *the diffusional method*, based on changing the original partial differential equation, instead of changing the numerical method, so that a self-adjoint form is obtained and leads to an optimal one-dimensional steady-state scheme;

– to show that the diffusional method can be naturally extrapolated to multidimensional problems;

– to analyse the range of applicability of a lumped capacitance matrix diffusional formulation;

– to investigate the possible use of the lumped form of the one-dimensional two-step Taylor–Galerkin scheme as a tool for solving transient non-linear equations and as a future tool for a one-step solver;

– to exemplify the associated performance of the transient schemes by means of the solution of two linear transient problems and Burger's non-linear equation;

– to present and compare explicit and implicit time-adaptive finite element procedures for solving linear and non-linear one-dimensional convection-diffusion equations, based on the diffusional method, the TSTG-α (lumped) scheme and literature available finite difference adaptive integrators.

2. BACKGROUND

The transient one-dimensional convection-diffusion equation can be written in the non-conservative form as

$$\frac{\partial \widehat{\phi}}{\partial t} + u\,\frac{\partial \widehat{\phi}}{\partial x} - \frac{\partial}{\partial x}\,\Gamma\,\frac{\partial \widehat{\phi}}{\partial x} + Q = 0 \qquad (1)$$

where $\widehat{\phi}$ is the dependent variable, and Q, u and Γ may depend on $\widehat{\phi}$, t and x.

2.1. Steady-state finite element one-dimensional solutions

The dependent variable $\widehat{\phi}$ is approximated, as usual, by means of

$$\widehat{\phi} \approx \phi = \boldsymbol{N}\boldsymbol{\phi} = \sum N_i\,\phi_i \qquad (2)$$

where $\boldsymbol{N}(\equiv N_i)$ is the shape function, ϕ the approximate value for $\widehat{\phi}$ and $\boldsymbol{\phi}(\equiv \phi_i)$ are the nodal points (vector).

The *variational* and *Petrov-Galerkin* methods are quoted in the literature to be *optimal* methods when applied to the one-dimensional steady-state convection-diffusion equation. Because of their importance in this work, they will be briefly reviewed. On the other hand

it is well known that Galerkin's formulation leads to oscillatory results as the local Péclet number increases above 2 [12] and will not be considered at this point.

For the present, Q, u and Γ *are assumed to be constant.* Given the weighting function $\boldsymbol{W}$ and the domain $0 \leq \times \leq L$, the *variational approach* is based on determining $p = p(x)$, so that

$$\int_0^L \boldsymbol{W}_{\mathrm{p}} \left[u \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \Gamma \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} + Q \right] \mathrm{d}x = 0 \qquad (3)$$

becomes self-adjoint. By making use of the associated weak formulation, the above equation (3) is written as:

$$\int_0^L \left[\boldsymbol{W} \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} \left(p\,u + \Gamma \frac{\mathrm{d}p}{\mathrm{d}x} \right) + \frac{\mathrm{d}\boldsymbol{W}}{\mathrm{d}x} \Gamma_{\mathrm{p}} \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} + \boldsymbol{W}_{\mathrm{p}}\, Q \right] \mathrm{d}x + \boldsymbol{W}_{\mathrm{p}}\, \Gamma \left. \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} \right|_0^L = 0 \qquad (4)$$

By forcing the convective term of the resulting integral to be zero, one arrives at:

$$p = p_0\, \mathrm{e}^{-2\,P\,x/L} \qquad (5)$$

where P = global Péclet number $= u\,L/2\,\Gamma$ and p_0 is a constant.

If a (Bubnov-)Galerkin formulation is applied ($\boldsymbol{W} = N_i$) equations (4) and (5) lead to:

$$\int_0^L \left[\frac{\mathrm{d}N_i}{\mathrm{d}x} \left(\Gamma\, \mathrm{e}^{-2\,P\,x/L} \right) \frac{\mathrm{d}N_i}{\mathrm{d}x}\, \widehat{\phi}_j + N_i\, \mathrm{e}^{-2\,P\,x/L}\, Q \right] \mathrm{d}x = 0 \qquad (6)$$

Assume N_i to be the linear interpolating functions and consider the discretization nodes $i-1$, i and $i+1$, whose co-ordinates are, respectively, x_{i-1}, x_i and x_{i+1}, such that the step size is $h = x_i - x_{i-1} = x_{i+1} - x_i$. In order to eliminate the difficulties associated with the numerical integration of the above equation [51–52], define p using an origin at $x = x_i$, and a *local Péclet number*, $Pe = u\,h/2\,\Gamma$, and, thus, equation (6) becomes:

$$\int_{-h}^{h} \left[\frac{\mathrm{d}N_i}{\mathrm{d}x} \left(\Gamma\, \mathrm{e}^{-2\,Pe\,x/h} \right) \frac{\mathrm{d}N_j}{\mathrm{d}x}\, \phi_j + N_i\, \mathrm{e}^{-2\,Pe\,x/h}\, Q \right] \mathrm{d}x = 0 \qquad (7)$$

leading, after integration, to the nodal equation,

$$a_{\mathrm{s}}\, \phi_{i-1} + b_{\mathrm{s}}\, \phi_i + c_{\mathrm{s}}\, \phi_{i+1} + d_i = 0 \qquad (8)$$

where

$$a_{\mathrm{s}} = 1 - \mathrm{e}^{2\,Pe}; \qquad b_{\mathrm{s}} = \mathrm{e}^{2\,Pe} - \mathrm{e}^{-2\,Pe};$$
$$c_{\mathrm{s}} = -1 + \mathrm{e}^{-2\,Pe}; \quad d_i = \frac{Q\,h^2}{2\,Pe\,\Gamma} \left(\mathrm{e}^{Pe} - \mathrm{e}^{-Pe} \right)^2 \qquad (9)$$

The *Petrov-Galerkin* [8] method consists in solving the steady-state convection–diffusion equation by means of the weighted residual integral:

$$\int_0^L \boldsymbol{W} \left[u \frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x} + Q \right] \mathrm{d}x = 0 \qquad (10)$$

where now the weighting function is given by:

$$\boldsymbol{W} = W_i = N_i + \overline{W}_i = N_i + \frac{\alpha\, h}{2} \frac{\mathrm{d}N_i}{\mathrm{d}x} \operatorname{sign}(u) \qquad (11)$$

where, for *optimal* solutions,

$$|\alpha| = \alpha_{\mathrm{opt}} = \coth|Pe| - \frac{1}{|Pe|} \qquad (12)$$

By substituting the above equation (12) in equations (10) and (11), a nodal equation of the same form as equation (8) is arrived at, with the following coefficients,

$$a_{\mathrm{s}} = -Pe\,(\alpha + 1) - 1; \quad b_{\mathrm{s}} = 2 + 2\,Pe\,\alpha;$$
$$c_{\mathrm{s}} = -Pe\,(\alpha - 1) - 1; \quad d_i = \frac{Q\,h^2}{\Gamma} \qquad (13)$$

If, in the above set of equations, α is taken as 0 or 1, the Galerkin or full upwind formulations are, respectively, obtained. The coefficients given by equation (9) are equivalent (after algebraic manipulations) to the ones given by equation (13), *mutatis mutandis.* Furthermore, the discontinuous nature of the weighting function $\overline{W}$ in the above equation (11) should also be noticed: $\overline{W}$ is assumed to be discontinuous within the element and, in this way, it is applied to evaluate only the convection term [8].

2.2. Transient finite element one-dimensional solutions

The following approximate equation, originated after spatial and one-step time discretization of the transient convection–diffusion equation, is classical:

$$\frac{\boldsymbol{C}\left(\phi^{n+1} - \phi^n\right)}{\Delta t} + \boldsymbol{K}\left[(1-\theta)\,\phi^n + \theta\,\phi^{n+1}\right] + \boldsymbol{D}^n = 0 \qquad (14)$$

where $0 \leq \theta \leq 1$; $\boldsymbol{C}$, $\boldsymbol{K}$ and $\boldsymbol{D}$ are, respectively, the capacitance, the conductivity (or stiffness) matrices and the force vector, and n is the time level. If the problem at hand is one-dimensional, if use is made of the terminology defined above for steady-state terms such as a_{s}, b_{s} and c_{s}, equations (8) and (9), and if new analogous transient coefficients are defined (with the subscript t), equation (14) can be rewritten in the form:

$$(a_{\mathrm{t}} + a_{\mathrm{s}}\,\theta)\phi_{i-1}^{n+1} + (b_{\mathrm{t}} + b_{\mathrm{s}}\,\theta)\,\phi_i^{n+1} + (c_{\mathrm{t}} + c_{\mathrm{s}}\,\theta)\,\phi_{i+1}^{n+1}$$
$$= -d_i + [a_{\mathrm{t}} - a_{\mathrm{s}}\,(1-\theta)]\,\phi_{i-1}^{n}$$
$$+ [b_{\mathrm{t}} - b_{\mathrm{s}}\,(1-\theta)]\,\phi_i^{n} + [c_{\mathrm{t}} - c_{\mathrm{s}}\,(1-\theta)]\,\phi_{i+1}^{n} \qquad (15)$$

For eventual comparisons, the transient terms of the variational formulation of the convection–diffusion

equation can be obtained by pre-multiplying all terms of equation (1) by the function $\boldsymbol{W}_{\mathrm{p}}$ so that [12]:

$$\int_0^L \boldsymbol{W}_{\mathrm{p}} \left[\frac{\partial \widehat{\phi}}{\partial t} + u \frac{\partial \widehat{\phi}}{\partial x} - \frac{\partial}{\partial x} \Gamma \frac{\partial \widehat{\phi}}{\partial x} + Q \right] \mathrm{d}x = 0 \quad (16)$$

Re-scaling the integration limits and shape functions as before, after integration and some algebra, one arrives at the following nodal terms applicable to transient problems:

$$a_{\mathrm{t}} = \frac{1}{C\,Pe} \left[1 - \mathrm{e}^{2\,Pe} + Pe\,(1 + \mathrm{e}^{2\,Pe}) \right];$$

$$b_{\mathrm{t}} = \frac{1}{C\,Pe} \left[\mathrm{e}^{2\,Pe} - \mathrm{e}^{-2\,Pe} - 4\,Pe \right];$$

$$c_{\mathrm{t}} = \frac{1}{C\,Pe} \left[\mathrm{e}^{-2\,Pe} - 1 + Pe\,(1 + \mathrm{e}^{-2\,Pe}) \right] \quad (17)$$

where $C = \dfrac{u\,\Delta t}{h}$ is the *local Courant or convection number*. Zienkiewicz and Taylor [12] showed that the above scheme, as applied to the variational scheme, is generally unstable. Only for $C \geq 1$ the fully implicit scheme leads to stable solutions. They also showed that the transient form of the Petrov–Galerkin method with optimal upwind performs better than the variational method, but shows excessive dampening for solving problems, except for very small Courant numbers. No further mention will be made of the transient Petrov–Galerkin scheme.

A special reference should be addressed to the second order Taylor–Galerkin scheme, originally proposed by Donea [22] and further modified to a two-step scheme, in a series of papers, by Löhner, Morgan and Zienkiewicz [23, 53] and co-workers. Donea's scheme can be obtained by expanding the dependent variable in a Taylor series in time, effectuating manipulations similar to the Lax–Wendroff finite difference scheme and finally applying a Galerkin approximation to the resulting time discretized formulation. Not going through the details, the explicit form of the two step Taylor–Galerkin, TSTG, scheme consists in obtaining a predictor equation for the dependent variable by neglecting the diffusion term so that the one-dimensional conservative form of equation (1) is approximated by

$$\phi^{n+1/2} = \phi^n - \frac{\Delta t}{2} \left[\frac{\partial (u\phi^n)}{\partial x} + Q \right] \quad (18)$$

From this predictor equation, one can estimate the convective flux, $(u\,\phi)^{n+1/2}$, and, finally, substitute this approximation into the corrector equation, that is, the Taylor–Galerkin scheme. This procedure is equivalent to a Galerkin formulation with the convective flux explicitly evaluated at $n + 1/2$. By neglecting the source term, the one-dimensional two-step scheme can be written as:

$$\frac{1}{3\,C}\,\phi_{i-1}^{n+1} + \frac{4}{3\,C}\,\phi_i^{n+1} + \frac{1}{3\,C}\,\phi_{i+1}^{n+1} - \left(1 + C + \frac{1}{Pe}\right)\phi_{i-1}^n + 2\left(C + \frac{1}{Pe}\right)\phi_i^n + \left(1 - C - \frac{1}{Pe}\right)\phi_{i+1}^n = 0 \quad (19)$$

which should be compared with the scheme obtained from the standard explicit Galerkin transient formulation,

$$\frac{1}{3\,C}\,\phi_{i-1}^{n+1} + \frac{4}{3\,C}\,\phi_i^{n+1} + \frac{1}{3\,C}\,\phi_{i+1}^{n+1} - \left(1 + \frac{1}{Pe}\right)\phi_{i-1}^n + \frac{2}{Pe}\,\phi_i^n + \left(1 - \frac{1}{Pe}\right)\phi_{i+1}^n = 0 \quad (20)$$

The TSTG scheme does not normally reduce to the Petrov–Galerkin scheme under steady-state conditions, and, therefore, the scheme is not applicable to problems involving boundary layers. However it does apply to a broad class of transient problems involving travelling waves (with or without diffusion) and pollutant dispersion [24].

3. A NEW CONCEPT: THE DIFFUSIONAL METHOD

The following points should be noticed:

– the optimality of the Petrov–Galerkin, PG, formulation was proven only for the case of one-dimensional steady-state convection-diffusion equation;

– although important advances have been made [8–10], extending the above variational and PG formulations to two and three-dimensional problems is rather cumbersome, if optimality is at stake.

A methodology is now proposed which is, at the same time, both natural and extendible to multidimensional problems. Undoubtedly, if the method to be proposed is correct, it should agree with both formulations (variational or Petrov–Galerkin) shown above since they lead to exact solutions. Besides, one should consider that it is well known that the Galerkin FE method leads to a best approximation ϕ to the exact solution $\widehat{\phi}$ of linear diffusion equations [12, 54, 55], in the sense that the nth derivatives of ϕ best fit the nth derivative of $\widehat{\phi}$ with respect to the energy norm. This extremely basic and well-established assertion (theorem) will serve as one of the bases for this work.

Based on the just exposed reasoning, *let us accept and use the obvious fact that linear and non-linear Diffusion Problems (elliptic and parabolic problems) can, in general, and in the absence of strong non-linearities, be accurately solved by means of any of the classical numerical methods, that is, Finite Differences, Finite Elements and Finite Volumes*, and simply transform equation (1) into a diffusion equation by letting

$$u \frac{\partial \widehat{\phi}}{\partial x} - \frac{\partial}{\partial x} \Gamma \frac{\partial \widehat{\phi}}{\partial x} = A \frac{\partial}{\partial x} \Gamma B \frac{\partial \widehat{\phi}}{\partial x} \quad (21)$$

Thus:

$$A\,\Gamma\frac{\partial B}{\partial x}=u;\quad A\,B=-1\Rightarrow B=B_0\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x} \tag{22}$$

where B_0 is a constant. The lower limit of integration can be changed in the above equation (22). Equations (1), (21) and (22) lead to the one-dimensional transient diffusional form of the convection-diffusion equation (CDE).

3.1. One-dimensional transient diffusional form of the convection-diffusion equation (CDE)

$$\frac{\partial\widehat{\phi}}{\partial t}-\mathrm{e}^{\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}\frac{\partial}{\partial x}\left(\Gamma\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}\frac{\partial\widehat{\phi}}{\partial x}\right)+Q=0 \tag{23}$$

Numerical techniques applied to equation (23) will (probably) fail since the original form of equation (1) will be restored. In order to avoid this fact, let us simply change equation (23) into another equivalent form.

3.2. General one-dimensional diffusional form of the CDE

$$\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}\frac{\partial\widehat{\phi}}{\partial t}-\frac{\partial}{\partial x}\left(\Gamma\,\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}\frac{\partial\widehat{\phi}}{\partial x}\right)+\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}Q=0 \tag{24}$$

If one assumes u/Γ to be constant or an average within the integration range, then the above equation can be written in terms of the global Péclet number, P, as the simplified one-dimensional diffusional form of the CDE.

3.3. Simplified one-dimensional diffusional form of the CDE

$$\mathrm{e}^{-2\,P\,x/L}\frac{\partial\widehat{\phi}}{\partial t}-\frac{\partial}{\partial x}\left(\Gamma\,\mathrm{e}^{-2\,P\,x/L}\frac{\partial\widehat{\phi}}{\partial x}\right)+\mathrm{e}^{-2\,P\,x/L}\,Q=0 \tag{25}$$

The above equations (24–25) are in an excellent form, suited to be solved by any numerical technique, and more particularly, by the finite element method. They are already in *full and natural variational forms* and also show *Petrov-Galerkin-like weighting functions* multiplying the transient and source terms.

The above concepts can be easily extended to two and three dimensions. Again, for simplicity, only the expanded two-dimensional forms of the diffusional form of the convection-diffusion equation are presented.

3.4. General two-dimensional diffusional form of the CDE

$$\begin{aligned}&\mathrm{e}^{-\left[\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x+\int_0^y\frac{v}{\Gamma}\,\mathrm{d}y\right]}\left[\frac{\partial\widehat{\phi}}{\partial t}+Q\right]\\&-\mathrm{e}^{-\int_0^y\frac{v}{\Gamma}\,\mathrm{d}y}\frac{\partial}{\partial x}\left(\Gamma\mathrm{e}^{-\int_0^x\frac{v_i}{\Gamma}\,\mathrm{d}x_i}\frac{\partial\widehat{\phi}}{\partial x}\right)\\&-\mathrm{e}^{-\int_0^x\frac{u}{\Gamma}\,\mathrm{d}x}\frac{\partial}{\partial y}\left(\Gamma\,\mathrm{e}^{-\int_0^y\frac{v}{\Gamma}\,\mathrm{d}y}\frac{\partial\widehat{\phi}}{\partial y}\right)=0\end{aligned} \tag{26}$$

3.5. Simplified (constant property) two-dimensional diffusional form of the CDE

$$\begin{aligned}&\mathrm{e}^{-\left[2\,P_x\frac{x}{L_x}+2\,P_y\frac{y}{L_y}\right]}\left[\frac{\partial\widehat{\phi}}{\partial t}+Q\right]\\&-\mathrm{e}^{-2\,P_y\frac{y}{L_y}}\frac{\partial}{\partial x}\left(\Gamma\,\mathrm{e}^{-2\,P_x\frac{x}{L_x}}\frac{\partial\widehat{\phi}}{\partial x}\right)\\&-\mathrm{e}^{-2\,P_x\frac{x}{L_x}}\frac{\partial}{\partial y}\left(\Gamma\mathrm{e}^{-2\,P_y\frac{y}{L_y}}\frac{\partial\widehat{\phi}}{\partial y}\right)=0\end{aligned} \tag{27}$$

where P_x is the global x-Péclet number ($=u\,L_x/2\,\Gamma$); L_x is any characteristic length in the x direction; $P_y=v\,L_y/2\,\Gamma$ and L_y are defined mutatis mutandis.

Some consequences of the above concepts, which are extremely simple in essence, but, at least in the authors' conception, of broad applications, are the following.

– Equations (24–27) were obtained in a natural way, without any assumptions whatsoever concerning a numerical scheme. In other words, the above formulation is independent of the numerical scheme and can be handled by finite element, finite volume and finite difference techniques.

– The above equation (24) can be applied to linear or non-linear problems, compressible or incompressible flows; similarly, equation (25) can be applied to constant, locally constant or element-averaged Pe problems.

– The cited equations, after a simple Galerkin formulation, reduce to both the variational and Petrov-Galerkin formulations, when one-dimensional problems are considered.

– Evidently equations (24–27) could be claimed to be in a *variational form*; however this nomenclature *variational* is not used by other numerical methods and, thus, the proposed formulation of *diffusional form* supersedes the terminology of variational.

– *Close examination of equation (27) will show why two-dimensional Petrov-Galerkin and Variational Methods*

have not worked for two and three-dimensional problems: one single weighting function would not lead to an expression equivalent to equation (27)!

– The diffusional method can also be applied in conjunction with any order of interpolation polynomials used in finite element analysis.

4. A HYPERBOLIC SCHEME FOR THE ONE-DIMENSIONAL TRANSIENT CONVECTION-DIFFUSION EQUATION

From equation (17), after the same algebraic manipulations that can transform equation (9) to equation (13), the following, hereby defined, *hyperbolic* transient terms can be obtained (α is defined in equation (12)):

$$\begin{aligned} a_t &= \frac{\alpha}{C}\,[Pe\,(\alpha+1)+1];\\ b_t &= -\frac{2}{C}\,[Pe\,(\alpha^2-1)+\alpha];\\ c_t &= \frac{\alpha}{C}\,[Pe\,(\alpha-1)+1] \end{aligned} \tag{28}$$

Obviously both the hyperbolic (as described above) and exponential (equation (17)) approaches lead to the same solutions since they are equivalent. The hyperbolic model is easier to apply than the exponential counterpart since the formalism does not involve exponentiation. Furthermore, simplifications such as the following (among others) can be applied:

$$\alpha \approx \left(1-\frac{1}{|Pe|}\right)\,\mathrm{sign}(Pe), \tag{29}$$

with at least five significant figures if $|Pe| \geq 6$

and

$$\alpha \approx \frac{Pe}{3}, \tag{30}$$

with at least five significant figures if $|Pe| \leq 0.1$

If variable sized elements and/or variable coefficients are used, the coefficients shown in the *table* are obtained. In the *table*, the associated local Pe, C and Γ are assumed to be averages of the respective element nodal values. The coefficient associated to a constant source term Q is d_s ($d_i = d_s\,Q$).

5. THE PREVAILING MAIN GRID SCHEME - PMGV

The capacity (mass) lumping process, based both on the integral formulation of energy, mass and momentum (conservation) equations and on a parallel and well established procedure employed by the finite volume schemes [1] will be used in this work. Thus, for the time derivative (accumulation rate) term, let us assume that *the grid point value at i prevails*, such that:

$$\begin{aligned} \phi_{\mathrm{prec.}} &\approx [N_{i-1}\ N_i]\left\{\begin{matrix}\phi_i\\ \phi_i\end{matrix}\right\} = [N_{i-1}\ N_i]\left\{\begin{matrix}\widetilde{\phi}_{i-1}\\ \phi_i\end{matrix}\right\};\\ \phi_{\mathrm{suc.}} &\approx [N_i\ N_{i+1}]\left\{\begin{matrix}\phi_i\\ \phi_i\end{matrix}\right\} = [N_i\ N_{i+1}]\left\{\begin{matrix}\widehat{\phi}_i\\ \phi_{i+1}\end{matrix}\right\} \end{aligned} \tag{31}$$

where *prec* and *suc* mean the elements that include, respectively, the i and $i-1$ nodes, and the i and $i+1$ nodes; thus, $\widetilde{\phi}$ with any subscript always denotes the ϕ value at node i. This assumption (approximation) leads to the following form for the time derivative term:

$$\int_{-h}^{h} N_i\,\mathrm{e}^{-\int_0^x \frac{u}{\Gamma}\,\mathrm{d}x}\,\frac{\partial\phi}{\partial t}\,\mathrm{d}x \approx \int_{-h}^{h} N_i\,\mathrm{e}^{-\int_0^x \frac{u}{\Gamma}\,\mathrm{d}x}\,N_j\,\mathrm{d}x\,\frac{\mathrm{d}\widetilde{\phi}_j}{\mathrm{d}t} \tag{32}$$

This time derivative term can be integrated resulting in just one extra term (b_t) to be used in the resulting transient one-dimensional schemes. In this case, a_t and c_t are set equal to zero. Another way to obtain the new transient coefficients is simply to add the *old* values given in equation (17) and (28); this procedure leads to:

$$\begin{aligned} b_{t,\mathrm{new}} &= a_{t,\mathrm{old}} + b_{t,\mathrm{old}} + c_{t,\mathrm{old}},\\ a_{t,\mathrm{new}} &= 0 \quad \text{and} \quad c_{t,\mathrm{new}} = 0 \end{aligned} \tag{33}$$

Now, equation (15) changes into

$$a_s\,\phi_{i-1} + (b_t\,\phi_i + b_s\,\phi_i) + c_s\,\phi_{i+1} + d_i = 0 \tag{34}$$

leading to the PMGV scheme:

$$\begin{aligned} &a_s\,\theta\,\phi_{i-1}^{n+1} + (b_t + b_s\,\theta)\phi_i^{n+1} + c_s\,\theta\,\phi_{i+1}^{n+1}\\ &= -d_i - a_s(1-\theta)\phi_{i-1}^{n} + (b_t - b_s\,(1-\theta))\ \phi_i^n - c_s\,(1-\theta)\,\phi_{i+1}^n \end{aligned} \tag{35}$$

The new b_t value equals $d_s/\Delta t$. *The above equation (35) shows clearly the great advantage of using the PMGV scheme: if an explicit scheme is used, the capacitance matrix is diagonalized and no solver is required for obtaining the new ϕ values!*

5.1. Performance analysis of the PMGV scheme

Consider the linear one-dimensional convection-diffusion equations obtained by making $Q = 0$ in equation (1), and assuming u and Γ to be constant:

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} - \Gamma\,\frac{\partial^2\phi}{\partial x^2} = 0 \tag{36}$$

The exact solution to equation (36) is:

$$\widehat{\phi} = \phi_0 \, \mathrm{e}^{-\Gamma k^2 t} \, \mathrm{e}^{\mathrm{I}k(x-ut)} \tag{37}$$

which is the complex Fourier component for a single wave. In this equation, $I = \sqrt{-1}$, ϕ_0 is an arbitrary constant, and k is the wave number, related to the wavelength ℓ by: $\ell = 2\pi/k$.

The *amplification factor* $\widehat{G}$ is, by definition, given by:

$$\widehat{G} = \frac{\widehat{\phi}(t+\Delta t)}{\widehat{\phi}(t)} = |\widehat{G}| \, \mathrm{e}^{\mathrm{I}\lambda} \tag{38}$$

Applying equation (37) in this definition leads to the expressions for the *modulus* and *argument* of $\widehat{G}$, respectively given by:

$$|\widehat{G}| = \mathrm{e}^{-\Gamma k^2 \Delta t} = \mathrm{e}^{-(2\pi)^2 F \left(\frac{h}{\ell}\right)^2}$$

and $$\lambda = -k\,u\,\Delta t = -k\,C\,h = -2\pi C \frac{h}{\ell} \tag{39}$$

where $F = \Gamma \Delta t / h^2$ is the local *Fourier number or diffusion number* and the ratio ℓ/h gives the number of wavelengths contained in the element of length h. Equation (37) or (39) shows that in the case of pure convection ($\Gamma = 0$ or $Pe = \infty$) the exact solution consists of a travelling undampened ($|\widehat{G}| = 1$) wave. In the case of pure diffusion ($u = 0$), the exact solution is a decaying exponential with zero phase or argument ($\lambda = 0$). In addition, the following expression relating F, C and Pe holds: $Pe = C/2F$.

The von Neumann method [2–4, 56] was used to accomplish a stability analysis of the proposed PMGV scheme. By this method:

– the boundary conditions are assumed to be periodic;

– the exact nodal solution, $\widehat{\phi}_i^n$, at time t (or time level n), of the *finite element scheme* is obtained from the following expressions for the general Fourier component of the complex Fourier series representation of its exact spatial distribution:

$$\widehat{\phi}_i^n = \mathrm{C}\mathrm{e}^{\mathrm{I}\,i\,k\,h} \text{ and, thus, } \widehat{\phi}_{i\pm i}^n = \mathrm{C}\mathrm{e}^{\mathrm{I}\,(i\pm 1)\,k\,h} = \widehat{\phi}_i^n \, \mathrm{e}^{\pm \mathrm{I}\,i\,k\,h} \tag{40}$$

– the amplification factor for the classical one-step scheme, equation (15), is given by:

$$G = \frac{\phi_i^{n+1}}{\phi_i^n} = \frac{a_n \, \mathrm{e}^{-\mathrm{I}\,i\,k\,h} + b_\mathrm{n} + c_\mathrm{n} \, \mathrm{e}^{\mathrm{I}\,i\,k\,h}}{a_{n+1} \, \mathrm{e}^{-\mathrm{I}\,i\,k\,h} + b_{n+1} + c_{n+1} \, \mathrm{e}^{\mathrm{I}\,i\,k\,h}} \tag{41}$$

where:

$$a_n = a_\mathrm{t} - a_\mathrm{s}\,(1-\theta); \quad b_\mathrm{n} = b_\mathrm{t} - b_\mathrm{s}\,(1-\theta); \quad c_\mathrm{n} = c_\mathrm{t} - c_\mathrm{s}(1-\theta) \tag{42}$$

$$a_{n+1} = a_\mathrm{t} + a_\mathrm{s}\,\theta; \quad b_{n+1} = b_\mathrm{t} + b_\mathrm{s}\,\theta; \quad c_{n+1} = c_\mathrm{t} + c_\mathrm{s}\,\theta \tag{43}$$

– from the ratio of the amplification factors, $G^* = G/\widehat{G}$, one can obtain the *amplitude ratio*, $|G^*|$, and *relative celerity*, λ^*, by means of the expressions:

$$|G^*| = \frac{|G|}{|\widehat{G}|} \quad \text{and} \quad \lambda^* = \frac{|\lambda|}{|\widehat{\lambda}|} \tag{44}$$

The closer the amplitude ratio and the celerity approach unity, the better is the performance of the numerical scheme. If the $|G^*| > 1$ the method is unstable; if $|G* \,| \neq 1$ implicit numerical diffusion occurs. If $\lambda^* \neq 1$ then phase distortion or implicit numerical dispersion occurs [4].

Values for amplitude ratios and relative celerities were obtained by means of a symbolic language program. Data referring to the *one-step hyperbolic scheme, OH*, employ the steady state and transient coefficients given by equations (13), (15) and (28) while those referring to the *PMGV model* make use of equations (13), (28) and (35).

Performance characteristics for *pure convection* are shown in *figures 1* and *2* for the two schemes. As previously pointed out by Zienkiewicz and Taylor [12], the variational, that is, the OHM scheme, does not lend itself to practical use since it is generally unstable. On the other hand, a drastic improvement in performance is noticed when the PMGV scheme is employed.

The following points should be noticed:

– the PMGV scheme is unconditionally stable for the implicit schemes and conditionally stable ($C \leq 1$) in the case of the explicit schemes;

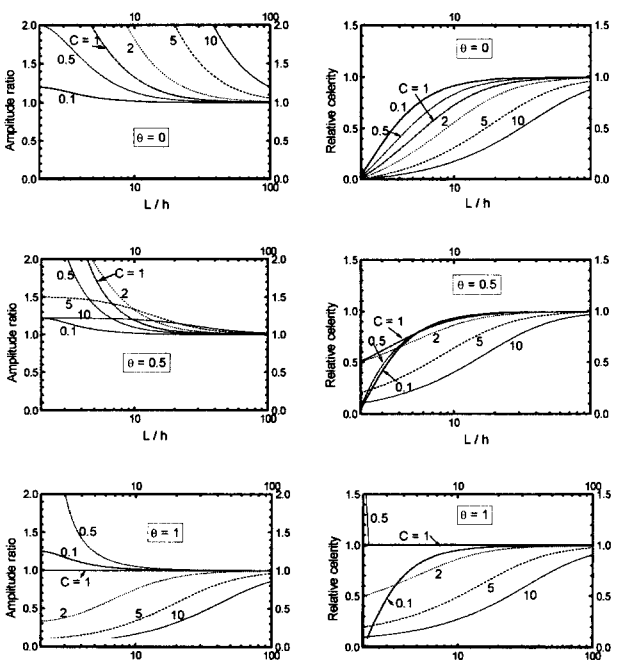


Figure 1. Performance characteristics of the hyperbolic scheme as applied to pure convection.

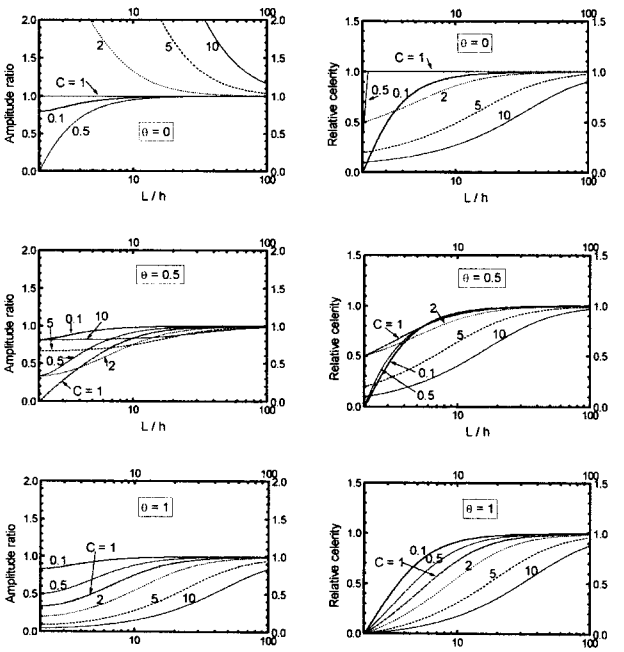


Figure 2. Performance characteristics of the PMGV scheme as applied to pure convection.

– the PMGV scheme shows a superior performance in terms of relative celerity, even for the *explicit scheme*, as long as $C \leq 1$;

– the PMGV scheme presents increasing dampening, as the scheme becomes more implicit (as θ increases); this dampening can, in principle, reduce its applicability to non-advection dominated flows; however it should be useful to obtain steady state solutions via transient solutions.

For *pure diffusion*, for stability ($G \leq 1$):

– if $\theta = 0$ and if F 0.5, then the PMGV is conditionally stable;

– if $\theta = 0.5$ or $\theta = 1$, the PMGV is unconditionally stable.

The performance of the PMGV scheme under *convection-diffusion* was analysed by means of symbolic programming; the main conclusions were:

– if $\theta = 0$ and if (but not necessarily) $F \leqq 1/4$, the PMGV is conditionally stable;

– if $\theta = 0.5$ or $\theta = 1$, the PMGV is unconditionally stable;

– if, in the explicit scheme, $F = 1/6$, then the order of the truncation error is $O(\Delta t^2) + O(\Delta x^2)$;

– once $F \leq 1/4$, the explicit scheme is convergent for all Pe; this is a very important conclusion, since as Pe increases, necessarily F decreases, and the limitation above is restricted to small Pe.

Consistency of equation (35) was investigated by expressing each of its terms in a Taylor series about the base grid point ϕ_i^n and comparing the resulting modified differential equation with the series expansion of the actual equation (37). The finite element scheme proved itself to be consistent with truncation error $O(\Delta t) + O(\Delta x^2)$. For completeness, this fact is confirmed by comparing the following Taylor series expansions of equations (38) (for all Pe) and (41) (for $\theta = 0$ and $Pe \to \infty$ only, due to the high complexity of the associated expansion):

$$\widehat{G} = 1 - I\,C\,\sigma - \frac{C}{2}\left(C - \frac{1}{Pe}\right)\sigma^2 + O(\sigma^3) \quad (45)$$

$$G = 1 - I\,C\,\sigma - 0.5\,C^2\,\sigma^2 + O(\sigma^3) \quad (46)$$

where $\sigma = 2\pi h/\ell$.

5.2. Lumped capacitance matrix scheme of the two-step Taylor-Galerkin (TSTG) scheme: the TSTG-α scheme

The two-step Taylor–Galerkin (TSTG) scheme is very effective; it is, however, limited to $C \leq 0.57$, in its explicit form [24, 25]; other Taylor–Galerkin (or characteristic) schemes may lead to increased stable ranges of C values [24, 25]. Peraire et al [24] show the destructive effect of a lumped capacitance matrix on a simple convection problem.

In this work, the lumped form of the TSTG scheme, from now on called the TSTG-α scheme, will have two main purposes:

– first, to show that the dissipative nature of the TSTG-α scheme decreases substantially as the mesh is refined and, thus, the resulting approximations approach definitely the results obtained from the application of the TSTG scheme.

– secondly, *to ascertain the fact that if in the PMGV scheme α (table) is replaced by C, the resulting scheme will perform identically to the TSTG-α scheme*; in other words:

Modified PMGV scheme or PMGV-α scheme
= TSTG-α scheme $\Rightarrow$ Make $\alpha = C$

in all coefficients shown in the *table*.

A *consistency* analysis shows that the above scheme is second-order accurate. Performance (stability) curves are shown in *figure 3a–b*. It is clearly shown that the modified model is stable for $C \leq 1$; in addition, it shows less dampening effect than the original PMGV, but is more dampening than the original TSTG scheme (see [25]).

The fundamental idea behind using the TSTG-α scheme is that by halving the spacing (h) value, the dampening effect is reduced; the cost of doubling the number of elements may be balanced by the increased allowed C-values and the associated diagonally full explicit scheme.

TABLE
Coefficients for the transient one-dimensional diffusional scheme.

a_s	$-\dfrac{h_{i+1}\left[Pe_{i+1}\left(\alpha_{i+1}+1\right)+1\right]}{\Gamma_{i+1}}$
c_s	$-\dfrac{h_i\left[Pe_i\left(\alpha_i-1\right)+1\right]}{\Gamma_i}$
b_s	$-(a_s+c_s)$
a_t	$\dfrac{\alpha_i\, a_s}{C_i}$
c_t	$-\dfrac{\alpha_{i+1}\, a_s}{C_i}$
b_t	$\dfrac{a_s}{C_i}\left[\alpha_i+Pe_i\left(\alpha_i-1\right)\right]$ $+\dfrac{c_s}{C_{i+1}}\left[\alpha_{i+1}-Pe_{i+1}\left(\alpha_{i+1}+1\right)\right]$
$d_s=(a_t+b_t+c_t)\,\Delta t$	$\dfrac{a_s\, h_i^2}{2\,\Gamma_i}\left(\alpha_i-1\right)-\dfrac{c_s\, h_{i+1}^2}{2\,\Gamma_{i+1}}\left(\alpha_{i+1}+1\right)$

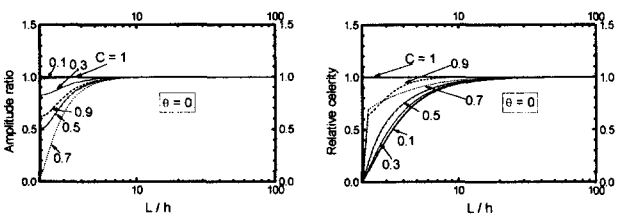


Figure 3. Performance characteristics of the TSTG-α scheme as applied to pure convection.

A series of examples, to be shown ahead, will serve to depict the behaviour of both the PMGV, in its explicit and implicit forms, and the TSTG-α schemes.

6. TIME ADAPTIVE SCHEMES

6.1. Bixler's implicit adaptive time integration scheme

As previously mentioned, Bixler [50] altered Gresho et al.'s [49] time integration scheme (GLS scheme) by incorporating modifications to enhance accuracy and stability. Given the first order differential equation (readily expandable to a system of ordinary differential equations):

$$\dot{y} = f(y,t) \tag{47}$$

Bixler's scheme consists basically in:

- using the second-order-accurate Adams-Bashforth scheme as predictor:

$$y_{n+1}^{p} = y_n + \frac{\Delta t_n}{2}\left[\left(2+\frac{\Delta t_n}{\Delta t_{n-1}}\right)\dot{y}_n - \frac{\Delta t_n}{\Delta t_{n-1}}\,\dot{y}_{n-1}\right] \tag{48}$$

where the superscript p refers to predicted value and the derivatives (rates of change) at time planes $n-1$ and n; $\dot{y}_{n-1}$ and $\dot{y}_n$ are respectively approximated by:

$$\dot{y}_{n-1} = \frac{\Delta t_{n-2}}{\Delta t_{n-1}+\Delta t_{n-2}}\left(\frac{y_n - y_{n-1}}{\Delta t_{n-1}}\right) + \frac{\Delta t_{n-1}}{\Delta t_{n-1}+\Delta t_{n-2}}\left(\frac{y_{n-1}-y_{n-2}}{\Delta t_{n-2}}\right) \tag{49}$$

and the trapezoid rule:

$$\dot{y}_n = \frac{2}{\Delta t_{n-1}}\left(y_n - y_{n-1}\right) - \dot{y}_{n-1} \tag{50}$$

- using the one-leg twin form of the trapezoid rule as corrector:

$$\frac{y_{n+1}+y_n}{\Delta t_n} = f\left(\frac{y_{n+1}+y_n}{2},\ \frac{t_{n+1}+t_n}{2}\right) \tag{51}$$

- predicting the time-step size by means of the expression:

$$\Delta t_{n+1} = \Delta t_n \left(\frac{\varepsilon}{|d_{n+1}^{*}|}\right)^{\frac{1}{3}}, \tag{52}$$

where

$$d_{n+1}^{*} = \frac{\beta}{2+\beta+3\,\Delta t_{n-1}/\Delta t_n}\left(y_{n+1}-y_{n+1}^{p}\right) \tag{53}$$

In the above equations n, $n-1$, $n-2$ and $n+1$ refer to time levels; $0 \le \beta \le 1$ is suggested to take the value 0.25 (if the GLS scheme is used, then $\beta = 1$; this is the choice in this work). Taking the superscript E to refer to the exact solution, the local time truncation error estimate relative to equation (48) can be obtained by means of Taylor series expansion as [49]:

$$y_{n+1} - y_{n+1}^{E} = \frac{1}{12}\,\Delta t_n^3\,\dddot{f}(y,t) + O(\Delta t^4) \tag{54}$$

Similarly, the local truncation error for equation (51) is given by [50]

$$y_{n+1} - y_{n+1}^{E} = \frac{\beta}{12}\,\Delta t_n^3\,\dddot{f}(y,t) + O(\Delta t^4) \tag{55}$$

Combination of the above two equations (54 and 55) allows one to obtain the time-step size, equation (52).

It should be noted that Bixler's scheme requires solutions at three preceding time- steps. Adaptive time

stepping can start at the fourth step. Furthermore, a norm such as the root means-square (RMS) should replace the absolute norm in equations (52 and 53) when a system of equations is to be solved.

6.2. Other integration formulas

Gresho et al. [49] suggested a scheme (GLS) using the explicit forward Euler (FE), as the predictor and, as the corrector, the implicit backward Euler (BE). For both the second and first-order schemes, GLS recommends the one-step Newton-Raphson method to solve the implicit correctors. Following GLS, the GLS-E scheme (E, for Euler), because of its dissipative nature, should be used only as a means for obtaining steady-state solutions.

Several other time adaptive integration techniques were investigated in a search for adequate adaptive integration techniques for both the explicit and implicit forms of the PMGV method. Among others, the following methods were tested:

(1) Adams-Bashforth predictor associated to the explicit Euler corrector: *AB-E scheme.*

(2) *Second order scheme: - modified-GLS (MGLS)*; here, instead of using equation (51), the explicit form (by making use of the predicted value) of the trapezoid rule was used as corrector; no use was made of the Newton–Raphson method. The rest of the procedures followed Bixler's method;

(3) first order schemes using mixed forms of Euler, Adams Bashforth and trapezoidal rules.

7. EXAMPLE PROBLEMS: TRANSIENT ONE-DIMENSIONAL LINEAR CONVECTION-DIFFUSION

7.1. Transient one-dimensional linear convection-diffusion

This example problem will serve to illustrate the behaviour of the PMGV scheme when applied to solve boundary layer problems. It was used by Hoffman [4] to illustrate the behaviour of several finite-difference numerical schemes applied to the convection-diffusion equation. The problem consists in solving equation (36) with the following boundary (Dirichlet) and initial conditions: $\phi(x,0) = x/L$, $\phi(0,t) = 0$ et $\phi(L,t) = 1$.

The analytical solution is:

$$\phi(x,t) = \frac{e^{\frac{P\,x}{L}} - 1}{e^{P} - 1} + \frac{4\,\pi\, e^{\frac{P\,x}{2\,L}} \sin\left(\frac{P}{2}\right)}{e^{P} - 1} \sum_{m=1}^{\infty} A_m + 2\,\pi\, e^{\frac{P\,x}{2\,L}} \sum_{m=1}^{\infty} B_m \quad (56)$$

where P is the global Péclet number and:

$$A_m = (-1)^m \frac{m}{\beta_m} \sin\left(\frac{m\,\pi\,x}{L}\right) e^{-\lambda_m t} \quad (57)$$

$$B_m = \left[(-1)^{m+1} \frac{m}{\beta_m}\left(1 + \frac{P}{\beta_m}\right) e^{-\frac{P}{2}} + \frac{m\,P}{\beta_m^2}\right] \cdot \sin\left(\frac{m\,\pi\,x}{L}\right) e^{-\lambda_m t} \quad (58)$$

$$\beta_m = \left(\frac{P}{2}\right)^2 + (m\,\pi)^2 \text{ and } \lambda_m = \frac{\Gamma\,\beta_m}{L^2} \quad (59)$$

The numerical results, obtained for $L = 1$, confirmed the previous performance analysis of the PMGV scheme. *Figure 4a* shows that the explicit scheme presents better accuracy than the implicit schemes. Even the explicit form of the PMGV scheme is not subject to any restrictions whatsoever on Pe; as Pe increases the restriction imposed on F, for stability, is reduced. *Figure 4b* shows that by decreasing the time step (C) the accuracy tends to increase as long as F gets smaller than 0.25; although results are shown only for $\theta = 0$, the same reasoning applies to the implicit schemes. It should be mentioned that, following [4], all nine of the most common finite difference schemes are not stable for $Pe \geq 1$ and are, in its heavy majority, restricted to $F \leq 0.5$, although their stability analysis might indicate otherwise. The PMGV scheme always converges to the exact values, independently of the Pe number, as long as the stability criteria are obeyed. Needless to say, large Courant numbers ($C > 1$) can be used with the implicit forms of the PMGV if only steady state solutions are aimed at. Additionally, but not exemplified for brevity, for all schemes, mesh refinement improves the accuracy.

The TSTG and TSTG-α schemes present time degrading and oscillatory steady-state solutions when Pe is larger than 1.5; the results resemble the ones presented by the standard Galerkin scheme and, thus, both schemes are not applicable to this type of problem, in the whole range from transient to steady-state conditions. For this reason, inherent example solutions are not shown.

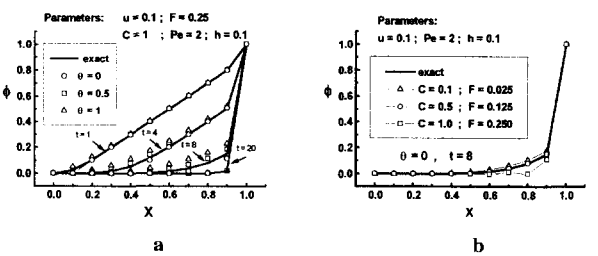


Figure 4. Solutions of the one-dimensional transient convection-diffusion equation; (**a**) comparison of explicit and implicit schemes; (**b**) effect of the Courant number on the numerical accuracy of the explicit scheme.

7.2. Transport of a Gaussian waveform

A rather 'classical' problem [12, 25, 28] is the pure convection of a waveform. Here the Gaussian distribution:

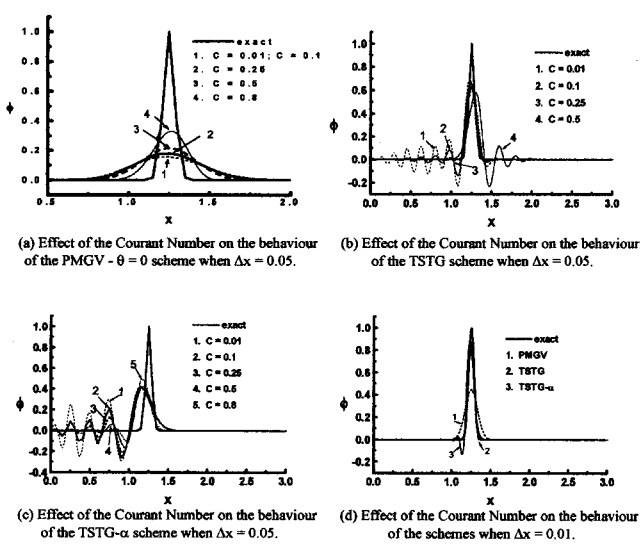
$$\widehat{\phi} = \mathrm{e}^{-400[x-u(1+t)]^2} \tag{60}$$

with $u = 0.25$, and $0 \leq x \leq 3$, was used to evaluate the performance of the different schemes under transient conditions with no boundary layers.

Figure 5 shows the behaviour of the different schemes. It can be observed that:

– the PMGV scheme is highly dissipative and should not be employed to solve this kind of problem. It should be noticed that as C increases (*figure 5a*), so does the performance of the PMGV scheme; thus, if high values of C and very fine meshes (*figure 5d*) can be used, the PMGV scheme, will be a choice to consider due to the fact that it does not show dispersion errors. However, problems involving such a situation are rare or expensive, but, as computer power increases, this might become an acceptable choice;

– the TSTG-α scheme shows much more dispersion and diffusion errors than the TSTG scheme (*figures 5b* and *5c*); in the case of the TSTG-α scheme, as C increases, the dispersion and the diffusion errors decrease and reach zero values at $C = 1$ (*figure 5c*); at low levels of refinement, the TSTG scheme, although presenting a definitively better performance than the TSTG-α, shows pronounced dispersion errors at low and close to its limiting upper C value of 0.57; its best performance is obtained for $C = 0.25$, at least for this travelling waveform example.



(a) Effect of the Courant Number on the behaviour of the PMGV - θ = 0 scheme when Δx = 0.05.

(b) Effect of the Courant Number on the behaviour of the TSTG scheme when Δx = 0.05.

(c) Effect of the Courant Number on the behaviour of the TSTG-α scheme when Δx = 0.05.

(d) Effect of the Courant Number on the behaviour of the schemes when Δx = 0.01.

Figure 5. Behaviour of the explicit PMGV, TSTG and TSTG-α schemes when applied to the pure waveform convection problem.

– if a more pronounced refinement is made (*figure 5-d*), at $C = 0.5$, both methods TSTG and TSTG-α, are highly acceptable; the trade-off concerning the more pronounced dispersion error of the TSTG-α scheme is the fact that it allows stable and accurate solutions up to $C = 1$ and a diagonalized capacitance matrix.

7.3. Solution of the viscous and non-viscous Burger's equation

Burger's equation is considered a benchmark, when non-linear convection-diffusion problems are considered. Now, solutions are presented for the viscous Burger's equation and its non-viscous form:

$$\frac{\partial \phi}{\partial t} + \phi \frac{\partial \phi}{\partial x} - \Gamma \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{61}$$

with the following boundary and initial conditions: $\phi(0,t) = 1$; $\phi(x,0) = 0$; $\phi(\infty,t) = 0$.

The solution of this problem is available [30, 31]; one solution, valid for large times (asymptotic), is [3]:

$$\phi = \frac{1}{1 + \mathrm{e}^{\left[\frac{x - 0.5\,t}{4\,\Gamma}\right]}} \tag{62}$$

Computer simulations revealed that the behaviour of all three schemes, but, more sensibly, the TSTG scheme, depend heavily on the Fourier number. The TSTG scheme has been known not to lead to inaccurate results when applied to solve Burger's equation; balancing diffusivities [57] and flux correction [53] have led to improved results. No such approximations were used in this work.

Again, computer experimentation and the results shown in *figure 6* (a–c) revealed that:

– when the F value was set to values above approximately 0.1, independently of $Re(= 1/\Gamma)$, the TSTG scheme presented oscillatory or highly diverged results; as F approached 0.1, the oscillations disappeared but the results showed waveforms advanced with respect to the exact solution;

– the PMGV and TSTG-α schemes led to accurate results, given the mesh refinement shown; Further mesh refinement led to even better results as can be seen in *figure 6c*; the PMGV scheme allows coarser refinement and does not show oscillatory results.

8. TIME ADAPTIVE FINITE ELEMENT SCHEMES FOR CONVECTION-DIFFUSION PROBLEMS

The same three different problems, two linear and one non-linear, involving convection-diffusion, pure

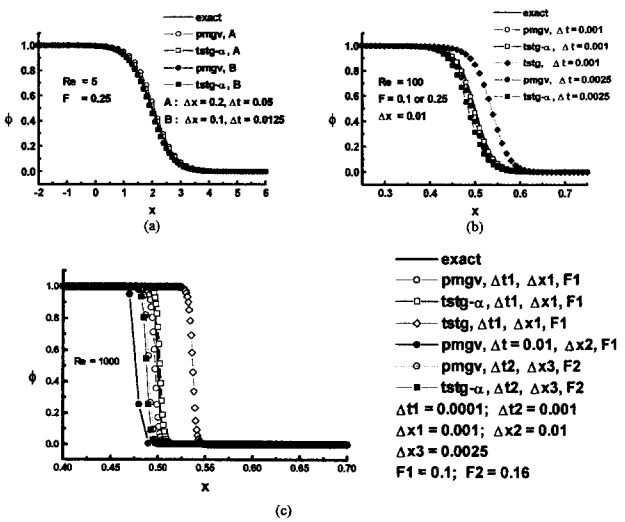


Figure 6. Solutions of Burger's viscous (a, b) and approximately non-viscous (c) equation under different schemes and time steps.

convection and non-linear Burger's equations were used to investigate the usefulness of the proposed adaptive schemes or part of them, as applied to the PMGV (diffusional), TSTG and TSTG-α schemes.

8.1. Transient one-dimensional linear convection-diffusion

Again, Hoffman's [4] example problem will serve to illustrate the behavior of the PMGV scheme when applied to solve boundary layer problems. Numerical solutions were investigated for Pe ranging from very small ($Pe = 0.05$) to pure convection ($Pe = \infty$). Numerical solutions were obtained by taking $L = 1$, $u = 0.1$, $\Delta x = 0.1$ and adjusting Γ so as to obtain the desired Pe value; the initial time step was taken as 10^{-3}.

A series of benchmark solutions showed that only the MGLS scheme was roughly competitive in relation to Bixler and the AB–E scheme; however it was discarded since it did not offer any advantage with respect to the AB–E scheme. The results obtained by means of the other methods showed that they were highly inefficient and, consequently, they will not be analysed here. Thus, in the discussion below, only Bixler and the AB–E schemes will be considered.

Figure 7 shows the simulation results for both Bixler and the AB-E schemes at $t = 7$. *Figure 7a* shows that the AB–E scheme led to exact results for *pure convection* when the truncation errors were $\varepsilon = 10^{-1}$ and 10^{-2}. This is due to the fact that at low truncation errors the time increment fast reached the value such that $C = 1$; at this Courant value, the explicit scheme leads to exact solutions. At the just cited truncation errors, 11 time levels were required to reach $t = 7$. Further decrease of the truncation error to 10^{-3} and 10^{-4} decreased the accuracy, while the number of time levels went up to 14 and 23 respectively. Bixler's method led to essentially the same results, independently of the assumed truncation error ($\varepsilon \leq 10^{-1}$); however, the required number of time levels increased substantially with a decrease of the assumed truncation error; in this way, n increased from 11 to 21 when ε decreased from 10^{-1} to 10^{-3}. Independently of the assumed truncation error, the AB-E scheme led to more accurate results than Bixler's.

At $Pe = 5$ (*figure 7b*), the AB-E scheme performs better when $\varepsilon = 10^{-3}$ and reaches time $t = 7$ within 14 time levels. The numerical results do not differ from the ones for pure convection. Again, as in the case of pure convection, the AB–E scheme is much more accurate than Bixler's. The accuracy of Bixler's scheme is insensitive to the assumed truncation error; in this case, the resulting solutions and required time levels do not differ from the ones obtained for pure convection.

At $Pe = 2$ (*figure 7c*) the accuracy of Bixler's scheme is again insensitive to the assumed truncation error. The AB-E scheme leads to more accurate results than Bixler's scheme, independently of the assumed truncation errors; its best accuracy is obtained for $\varepsilon = 10^{-4}$. At $Pe = 0.5$ (*figure 7d*), Bixler's scheme starts becoming more efficient both in terms of accuracy and required time levels for a given simulation time. The AB–E scheme required 23 and 15 time levels for $\varepsilon = 10^{-4}$ and 10^{-3}, respectively, while Bixler's scheme required 15 time levels when $\varepsilon = 10^{-3}$. For Pe values lower than $Pe = 0.5$, Bixler's scheme becomes much more efficient than the AB-E scheme.

Figure 8 shows the evolution of the standard deviations of the results obtained from Bixler and the AB-E schemes up to $t = 20$, which corresponds to approximate steady state conditions. The number of time steps (n)

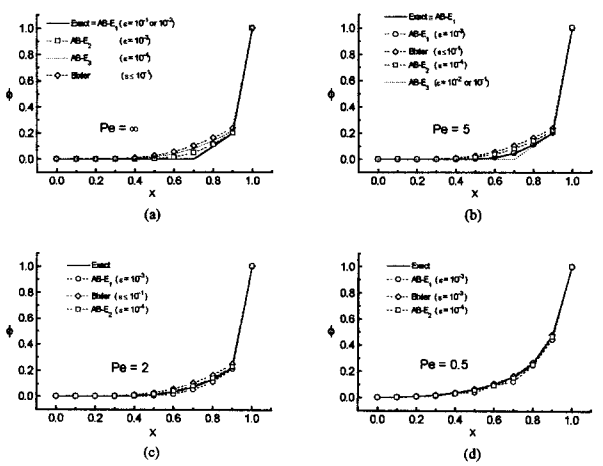


Figure 7. Solutions to the convection-diffusion equation, at $t = 7$.

required to reach $t = 20$ is also shown. It can be noted that as Pe decreases, Bixler's scheme becomes more and more efficient. However, the AB-E scheme works better as long as $Pe > 0.5$. It should also be noted that the AB-E scheme eliminates the restriction of $F < 0.25$ and $C < 1$, as can be seen in *figure 8f* (note that when $Pe = 0.5$, C and F are identical). However, if no control is made on the F values, specially at low Pe values, the standard deviation may show oscillatory results, as shown in *figure 8e*, where the F values went as high as 9.

Again, as in the case of non-adaptive procedures [58] and as seen before, the TSTG and TSTG-α schemes did not converge for Pe greater than 1.

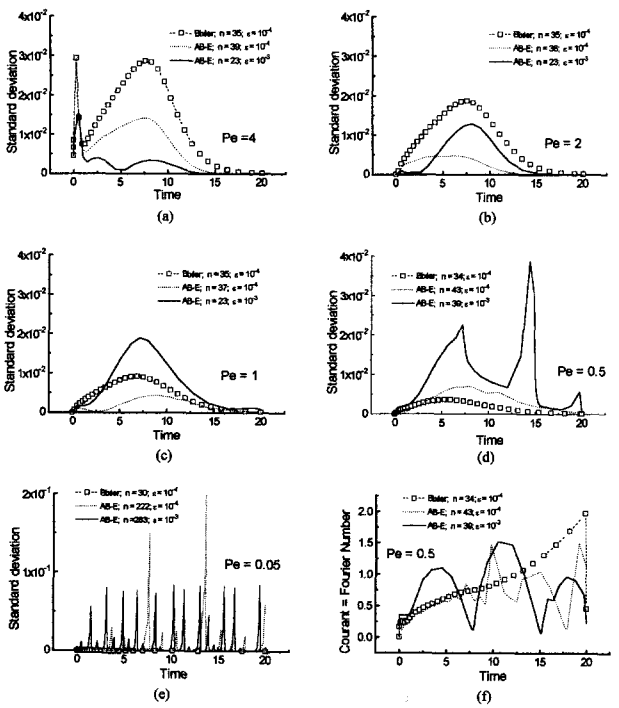


Figure 8. Standard deviation of Bixler and AB–E schemes up to $t = 20$.

Figure 9a shows how the TSTG scheme behaves, as a function of the 'assumed error', ε; the data were obtained for $\Delta x = 0.05$, and an initial time step of $\Delta t = 0.001$. It can be observed that as the error decreases, the numerical results tend to align with respect to the exact solution; at an error level of $\varepsilon = 10^{-3}$ oscillations are minimised. The cost of a better approximation is high, as can be noticed from the necessary number of time steps, n. *Figure 9b* shows that by increasing the error level ε the accuracy increases, for the given mesh refinement; when $\varepsilon = 0.1$, $n = 24$ and the numerical solution is very close to the analytical solution (and, consequently, is not shown). The effect of mesh refinement can be seen in *figures 9c–d*; in *figure 9d*, the results for $\varepsilon = 10^{-2}$ do not differentiate from the exact ones. As the mesh is refined, the numerical results become more accurate if $\varepsilon \leq 1^{-3}$ for the TSTG scheme and if $\varepsilon \geq 10^{-3}$ for the TSTG-α scheme. As a rule of thumb, the adaptive time refinement process is more efficient and accurate than the use of a constant time step; however, associated efficiency figures are sensitive to the scheme at hand, to the number of time steps as defined by the assumed error level, to the initial time step and, thus, are not shown.

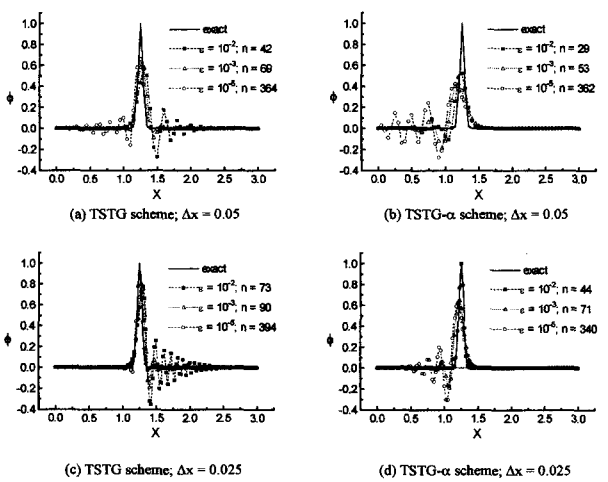


Figure 9. Performance of the TSTG and TSTG-α schemes as affected by assumed error levels.

8.2. Transport of a Gaussian waveform

Now, the problem of transport of a Gaussian wave was used to evaluate the performance of the TSTG and TSTG-α schemes under the time adaptive scheme obtained by using the Adams-Bashforth algorithm to generate the predictor, equation (48) and Bixler's time step updating formula, equation (51). As shown before in this work, the diffusional scheme is dissipative and should not be employed to solve travelling wave problems (unless Pe is very small, $Pe < 2$).

8.3. Solution of the viscous and non-viscous Burger's equation

Now Burger's equation is considered for the adaptive transient analysis.

Again, the simulated results shown in *figure 10* were obtained by assuming that the initial time step was 0.001, $Re = 1/\Gamma$ and the final simulation time was 1. *Figures 10a* (viscous condition) and *6d* (approximate non-viscous condition) show that, in the case of the

PMGV scheme, time adaptive integration by means of the AB-predictor adjustable time step leads to excellent results; it should be noticed that small ε values may result in oscillations. Adaptive time integration does not apply in an effective way to the TSTG-α scheme (*figure 10b*); however, a fixed time step procedure leads to good results. The TSTG scheme is not amenable to time adaptation and special shock capturing techniques should be employed, at higher Re values; even for $Re = 10$, strong oscillations appeared when $\varepsilon = 10^{-3}$.

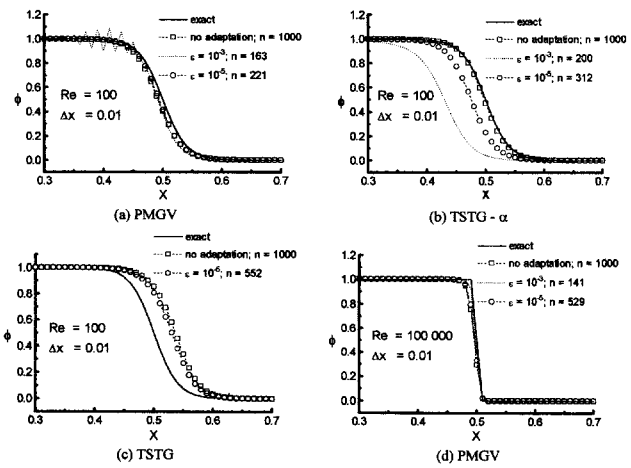


Figure 10. Solutions of Burger's viscous and non-viscous ($Re = 100\,000$) equation under different schemes.

9. CONCLUSIONS

This work presents a diffusional approach to solving the convection-diffusion equation that leads to the variational one-dimensional steady-state Galerkin formulation. The new concept for solving the convection-diffusion equations by means of a diffusional model can be extrapolated easily to multidimensional problems with no recourse to whatsoever ad-hoc improvements. In addition, further study was made on the performance of the one-dimensional lumped capacitance form of the diffusional method, which is equivalent to the variational method. Thus, the Prevailing Main Grid Value (PMGV) scheme is presented and it is shown to be unconditionally stable in its implicit forms and conditionally stable in its explicit form. The explicit form requires that $C \leq 1$; in addition, for low Pe, the Fourier number (F), should be $F \leq 1/4$. Differently from the usual finite difference schemes, all PMGV schemes converge for all Pe. Furthermore, the lumped one-dimensional form of the two step Taylor–Galerkin scheme was investigated as to its range of applicability.

Benchmark solutions involving boundary layer formation, travelling wave and Burger's equations were used in the analysis and as example problems. The main conclusions were:

- the PMGV scheme, both in its implicit and explicit forms apply to boundary layers transient problems and to solve the non-linear Burger's equations; consistently, the explicit form is more accurate; the PMGV scheme is not well suited to solve travelling wave problems;
- the TSTG-α scheme can be used to solve the non-linear Burger's equation accurately; however its range of F-values for non-oscillatory results is smaller than the ones applied to the PMGV scheme;
- both the TSTG and TSTG-α schemes do not apply to boundary layer transient problems, unless very small Pe and F numbers are used.

The performance of the diffusional method was also evaluated as to its adaptiveness by using it in association with a second-order Adams–Bashforth predictor and the implicit ($\theta = 0.5$–Bixler) and explicit (backward Euler or fully explicit) forms of the diffusional method were used as correctors. The main conclusions were that the explicit scheme (PMGV) is more accurate and computationally more efficient than the implicit (Bixler) version when applied to a linear boundary layer problem; for this problem the adaptive technique allowed overcoming the limitations of convection number, $F < 1/4$, and Courant number, $C < 1$. The time adaptive PMGV scheme proved to work very efficiently when solving Burger's equation, both under viscous and non-viscous conditions. The diffusional method is not well suited to travelling wave problems.

In addition, the performance of the one-dimensional form of the two-step Taylor–Galerkin (TSTG) scheme was investigated as to its ability to be used in conjunction with a time adaptive integrator. Both the explicit and fully lumped (TSTG-α) schemes work well under adaptive integration for solving linear travelling wave problems; for these problems, the TSTG scheme is more accurate than the TSTG-α one. Time adaptiveness, in terms of the proposed techniques presented in this work, are not recommended for both the TSTG and TSTG-α schemes, when one is interested in solving Burger's non-linear equation.

This work serves as an introduction to the application of the diffusional method to the solution of multidimensional problems, including Navier-Stokes problems.

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