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A Time Adaptive Scheme for the Solution of the Advection Equation in the Presence of a Transient Flow Velocity

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Abstract: A Fourier analysis conducted on both the spatial and the temporal discretizations of the governing partial differential equation shows that the Courant number as well as the time marching scheme have significant influences on the numerical behaviour of a Modified Least Squares (MLS) method for the solution of the advection equation. The variations of the amplification factor and the relative phase velocity with the Courant number and the dimensionless wave number indicate that when Courant number is equal to unity, the MLS method with the specified time-weighting and upwind function gives accurate results. This conclusion is confirmed by the numerical computation of the problem of the one-dimensional advective transport with constant flow velocity, carried out with different Courant numbers. Based on this observation, a time-adaptive scheme is developed to examine the problem where the advective transport has a time-dependent velocity. The time step is selected adaptively using the Courant number criterion $Cr = 1$. The time-adaptive scheme is applied to analyze the advective transport problem in which the flow velocity is governed by a pressure transient, resulting from the consideration of the compressibilities of the pore fluid and the porous skeleton, as well as the transient hydraulic boundary conditions.

keyword: Modified Least Squares method, Fourier analysis, advection equation, Courant number, time-adaptive scheme.

1 Introduction

The advection-diffusion equation can be used to model a wide range of problems in the engineering sciences. Examples of these include, waves in shallow water, heat transfer in fluids, salt movement in the oceans, flow of vehicular traffic, movement of charged particles such as electrons, gas dynamics, biological processes, tumor growth, sediment contamination of aquifers, and the transport of chemicals and other contaminants in porous geological media [Selvadurai (2000; 2002a; 2003)]. In general, the equations governing advective-diffusive transport are non-linear; the nonlinearities resulting largely from the modeling of the transport processes. The analytical solution of these equations is rarely possible. Therefore, it is necessary to employ computational methods to solve such transport problems of particular interest to engineering applications. In general, the computational solution of problems involving both advection and diffusion presents less computational difficulties than those that involve purely advective processes. Therefore, the development of reliable computational schemes that address the advective transport problem has been a challenging area of research in computational fluid dynamics. To date many studies have been made to develop stable numerical schemes with high accuracy for the solution of the advection equation, particularly in the presence of sharp gradients or discontinuities of the dependent variable [LeVeque (1992); Morton (1996); Quarteroni and Valli (1997); Ganzha and Vorozhtsov (1998); Wang and Hutter (2001); Atluri (2004)].

Many finite element methods, referred to as stabilized techniques, have been developed for the solution of the advection equation [Codina (1998)]. The main drawback of stabilized finite element methods, however, lies on their reliance on the well-established mesh discretization of the entire domain for the calculation of integral quantities. Such a limitation can be overcome by methods such as the Meshless Local Petrov-Galerkin (MLPG) method [Atluri and Zhu (1998); Atluri et al (2004)]. Recently, the MLPG technique has been applied to the solution of convection-diffusion problems [Lin and Atluri (2000)].

Most stabilized finite element methods satisfy the von Neumann stabilization condition, and based on Lax's equivalence theorem, the numerical solution will converge to a correct solution, provided consistent stability is

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observed. Since different stabilized methods use different weighting strategies, they are bound to have performances with varied accuracy for advective transport involving either discontinuities or a shock-structure in the solution. These differences in the numerical performance raise the question as to how rapidly the numerical solutions obtained by these stabilized schemes will converge to the true solution.

A Fourier analysis shows that a square wave is composed of waves of different frequencies, and the high frequency components can be considered as fine scale measures for which a simple polynomial space is inadequate. Therefore, the standard finite element space should be augmented by a space of functions (bubble functions) that take into consideration the effect of *discontinuous fronts*. The bubble functions should be specially constructed via a certain element-level homogeneous Dirichlet boundary value problem [Franca and Hwang (2002)], and therefore they are referred to as the *residual-free bubble*s [Brezzi, et al (1992); Franca and Farhat (1995)]. Another approach is to consider the effect of the *unresolvable fine scale* (or subgrid scale) on a *resolvable coarse* scale in the normal polynomial space by means of the elemental Green's function. This is the basic concept underlying the *variational multi-scale* model [Hughes (1995)]. Brezzi et al (1997) showed the equivalence of the *residual-free bubbles* approach and the *variational multi-scale* model for advection-dominated transport phenomena, and both approaches add a stabilization term to the weak form of the advection-diffusion operator [Codina (1998)].

Since the Fourier analysis can reflect a property of numerical schemes in the frequency domain, it has become one of the common ways to investigate the behavior of computational methods, particularly those that utilize the finite difference form of the advection equation [Morton, 1980; Pereira and Pereira, 2001]. Richtmeyer and Morton (1967) and Yu and Heinrich (1986) have used the amplitude ratio to investigate the stability of the space-time Petrov-Galerkin method; Shakib and Hughes (1991) presented a Fourier stability and accuracy analysis of the space-time Galerkin/least-squares method applied to the time-dependent advective-diffusive transport problem. Tezduyar and Ganjoo (1986) used the algorithmic damping ratio (ADR) and algorithmic frequency ratio (AFR) procedures to develop and test the weighting functions, which were used in an improved Petrov-Galerkin method. Codina (1993) used techniques involving both ADR and AFR to examine the stability of the forward-Euler scheme in the Streamline Upwind Petrov-Galerkin (SUPG) for the advection-diffusion equation. Cardle (1995) used a similar idea to determine the temporal weighting function, which is different from the spatial one utilized in the Petrov-Galerkin method. Recently, Hauke and Doweidar (2005) performed a Fourier analysis on a transient subgrid scale stabilized method for the advection-diffusion-reaction equation. These investigations suggest that the Fourier analysis provides considerable insight into the numerical behavior of stabilized methods for the solution of the advection equation. The overall behavior of stabilized finite element methods depends not only on temporal and spatial discretization schemes, but also on the form of the artificial diffusion and artificial convection introduced into the scheme through the numerical modeling. Therefore it is of interest to conduct Fourier analysis on all the discretization procedures simultaneously to examine the accuracy of the various numerical methods.

The main purpose of this paper is therefore to investigate the performance of stabilized semi-discrete Eulerian finite element methods via a Modified Least Squares scheme. Such an investigation is performed in terms of a Fourier analysis which is conducted on the discretization of both temporal and spatial derivatives of the advection equation. The trapezoidal time-weighting rule is considered in such a Fourier analysis and the influence of time-weighting on the numerical behavior of stabilized semi-discrete methods is identified by the distribution of algorithmic amplitude and relative phase velocity as a function of the dimensionless wave number and the Courant number. The upwind parameter and the time-weighting in the Modified Least Squares method are determined by means of a Fourier analysis to provide a greater accuracy in the amplification factor and relative phase velocity in terms of dimensionless wave number. The Fourier analysis also shows that the Courant number has a significant influence on the numerical performance of the above stabilized method, and therefore a time-adaptive scheme should be combined with the stabilized method to solve advective transport problems with a transient flow velocity. Finally, the time-adaptive Modified Least Squares method is used to examine the advective transport process in a porous medium, in which the flow is controlled by a transient flow potential.

Table 1 : The definition of upwind function for different methods

Methods	α_1	α_2
PG	$\frac{1}{\sqrt{15}}h$	$\frac{1}{\sqrt{15}}h$
LS	$\theta \lvert u \rvert \Delta t$	$\theta \lvert u \rvert \Delta t$
TG2	0	$\frac{1}{2} \lvert u \rvert \Delta t$
TG3	$\frac{1}{6} \lvert u \rvert^2 \Delta t^2 \frac{d}{dx}$	$\frac{1}{2} \lvert u \rvert \Delta t$
where h is the element length, Δt is time step and $Cr = \lvert u \rvert \Delta t / h$ is the elemental Courant number		

2 The Modified Least Squares Method

The basic concept underlying stabilized methods for examining computational modeling of the advection-dominated transport problem is to introduce artificial diffusion near the discontinuities of the dependent variable. The origins of such stabilized methods can be traced back to the combining of two basic finite difference methods: the central-difference scheme and the upwind-scheme. In this combination, the weighting of the upwind scheme should be increased near locations where the dependent variable has high gradients and in other regions the weighting of the central scheme should dominate. Therefore this method is referred to as an 'optimal' or 'smart' upwind method. Such smart upwind schemes can be introduced into finite element methods to develop the so-called stabilized semi-discrete Eulerian finite element methods, using asymmetric weighting functions [Christie et al (1976)]. The general weak form of the stabilized finite element method for the homogeneous advection equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{1}$$

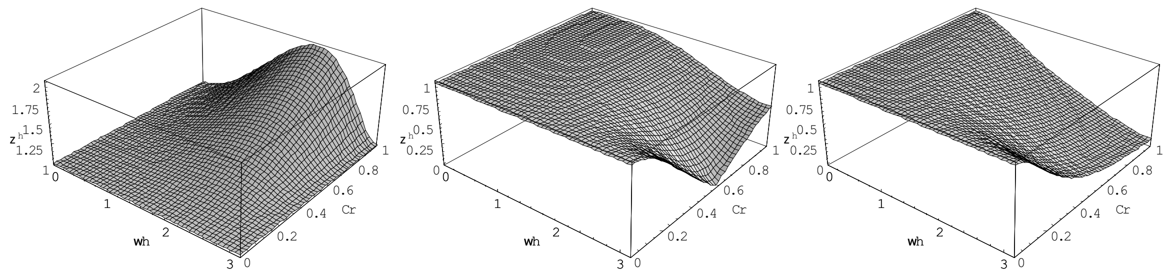
in a one-dimensional domain $\Omega(= [0,l])$ can be written as follows:

$$\int_\Omega \left[w + \alpha_1 sign(u)\frac{dw}{dx}\right]\frac{\partial C}{\partial t}\mathrm{d}x + \int_\Omega \left[w + \alpha_2\, sign(u)\frac{dw}{dx}\right](u\frac{\partial C^{n+\theta}}{\partial x})dx = 0 \tag{2}$$

where $C^{n+\theta}$=(1-θ)C^n+ θ C^{n+1}, $\theta \in$(0, 1] is time weighting, w is the standard Galerkin weighting function, α_i (i=1,2) are perturbation parameters referred to as the upwind functions or the intrinsic time of the stabilized methods [Oñate et al. (1997)]. The upwind functions should be determined on the basis of either the Least Squares method (LS) [Carey & Jiang (1988); Jiang (1998)] such that the artificial convection term has the adjoint form of the convection term in the equation which gives rise to symmetric computational schemes for the advection equation [Wendland & Schmid (2000)]; or be based on a Fourier analysis to ensure that numerical modelling can give an "optimal" solution of the transient advection-diffusion equation [Raymond & Garder (1976)], such as the Streamline Upwind Petrov-Galerkin Method (SUPG) [Hughes & Brooks (1982)]. Furthermore, the upwind functions can also take different values to generate different stabilized methods, such as the Taylor-Galerkin method (TG) [Donea et al. (1984)]. The expressions for the upwind functions, α_i (i=1,2), for several stabilized finite element methods, the Petrov-Galerkin method (PG), the Least Squares method (LS), the second- and the third-order Taylor-Galerkin methods (TG2 and TG3), are listed in Table 1.

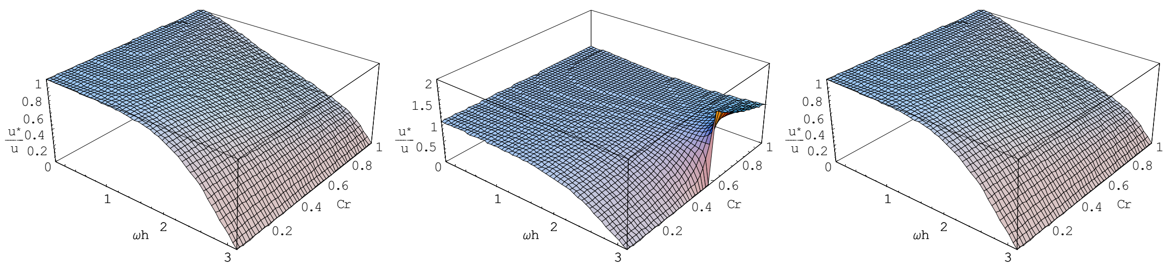
Since a Least Squares Method can generate a symmetric matrix form for the advection equation, the method has significant potential for the examination of the non-linear problem. Wendland and Schmid (2000) proposed a so-called 3S (Symmetrical Streamline Stabilization) scheme for advection-dominated transport, in which a parameter was introduced into the upwind term to obtain a better performance. This is equivalent to using different perturbation parameters for the temporal and spatial terms of the advection equation in the LS method: i.e.

$$\int_\Omega \left[w + \theta\, u\Delta t\frac{dw}{dx}\right]\frac{C^{n+1} - C^n}{\Delta t}dx + \int_\Omega \left[w + \alpha\theta\, u\Delta t\frac{dw}{dx}\right]u\frac{\partial C^{n+\theta}}{\partial x}dx = 0 \tag{3}$$



(a) θ=0.0 (b) θ=0.5 (c) θ=1.0

Figure 1 : The amplification factor for the MLS method for the advection equation with α=1; variation with ω*h* and *Cr*.



(a) θ=0.0 (b) θ=0.5 (c) θ=1.0

Figure 2 : The relative phase velocity for the MLS method for the advection equation with α=1; variation with ω*h* and *Cr*.

and this scheme can therefore be referred to as the Modified Least Squares method. The parameter α in (3) accounts for the upwind effect, which can be determined from a Fourier analysis to obtain the better numerical performance of the MLS method for the advection equation.

3 Fourier Analysis

The finite difference stencil for a Modified Least Squares method with a trapezoidal time-rule for the one-dimensional pure advection equation (1) can be written as

$$C_j^{n+1} = C_j^n + \Delta t[\theta \mathbf{A} C_j^{n+1} + (1-\theta)\mathbf{A} C_j^n] \tag{4}$$

where $\mathbf{A} = \mathbf{A}_1^{-1} \cdot \mathbf{A}_2$ and $\mathbf{A}_i (i = 1, 2)$ are discrete operators defined by

$$\mathbf{A}_1(C_j) = \frac{1}{6}(C_{j-1} + 4C_j + C_{j+1}) + \frac{\theta u \Delta t}{2h}(C_{j-1} - C_{j+1}) \tag{5a}$$

$$\mathbf{A}_2(C_j) = \frac{u}{2h}(C_{j+1} - C_{j-1}) - \frac{\alpha\theta\Delta t u^2}{h^2}(C_{j-1} - 2C_j + C_{j+1}) \tag{5b}$$

The sinusoidal form of the solution of (4) can be written as

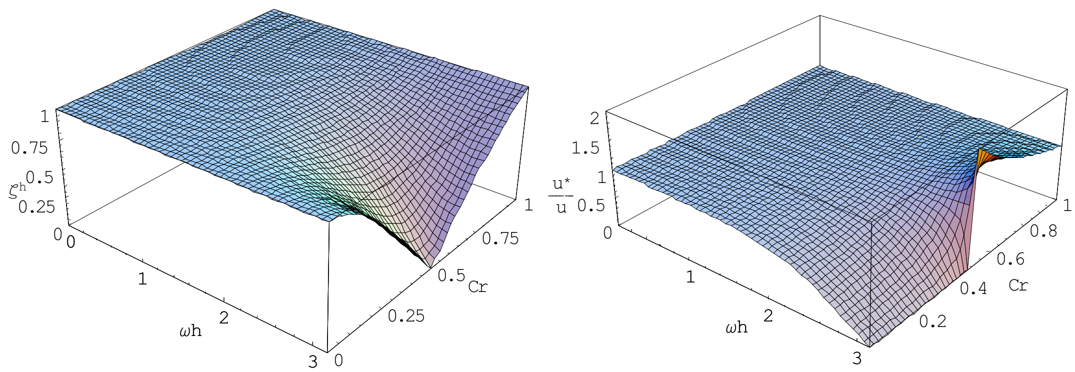
$$\begin{aligned} C_j^n = C(x_j, t_n) &= \exp[i\omega x_j - \nu^h t_n] \\ &= \exp[-\xi^h t_n]\exp[i\omega(x_j - \tfrac{\Omega^h}{\omega} t_n)] \end{aligned} \tag{6}$$

where $h = x_{j+1} - x_j$, $\Delta t = t_{n+1} - t_n$, ω is the spatial wave number, $\nu^h = \xi^h + i\Omega^h$ determines the temporal evolution of the solution, ξ^h and Ω^h are, respectively, the numerical damping coefficient and the wave frequency corresponding to the spatial increment h. Substituting (6) into (4) gives

$$[\zeta^h e^{-i\Omega^h \Delta t}]C_j^n = z(\omega) C_j^n \tag{7}$$

where ζ^h is the *amplification factor* for the numerical operator in (4) defined by

$$\zeta^h = \left| \frac{C_j^{n+1}}{C_j^n} \right| = \exp[-\xi^h \Delta t] \tag{8}$$



(a) Amplitude factor (b) Relative phase velocity

Figure 3 : The amplification factor and the relative phase velocity for the MLS method for the advection equation with α=3/2 and θ =1/3; variation with ωh and Cr.

and

$$z(\omega) = \frac{1+\Delta t(1-\theta)\hat{A}(\omega)}{1-\Delta t\theta\hat{A}(\omega)} = \frac{\left\{ \begin{array}{c} [2+\cos(\omega h)] - 6\alpha Cr^2\theta(1-\theta)\,[1-\cos(\omega h)] \\ -i\,3Cr\sin(\omega h) \end{array} \right\}}{[2+\cos(\omega h)] + 6\alpha Cr^2\theta^2[1-\cos(\omega h)]} \tag{9}$$

In (9), $\hat{A}(\omega)$ is the spectral function of the operator **A** [Vichnevetsky and Bowles (1982)].

From (7), (8) and (9), we can determine the amplification factor ζ^h and relative phase velocity u^*/u of the MLS method as follows:

$$\zeta^h = |z(\omega)| = \frac{\sqrt{\begin{array}{c}[2+\cos(\omega h) - 6\alpha Cr^2\theta(1-\theta)(1-\cos(\omega h))]^2 \\ +9Cr^2\sin^2(\omega h)\end{array}}}{2+\cos(\omega h)+6\alpha Cr^2\theta^2(1-\cos(\omega h))} \tag{10}$$

$$\frac{u^*}{u} = \frac{\Omega^h}{\omega} = -\frac{\arg(z(\omega))}{\omega\Delta t} = \frac{1}{Cr\,\omega h}\arctan\left(\frac{3Cr\sin(\omega h)}{\begin{array}{c}2+\cos(\omega h)\\ -6\alpha Cr^2\theta(1-\theta)(1-\cos(\omega h))\end{array}}\right) \tag{11}$$

Figures 1 and 2 illustrate, respectively, the variations in the amplification factor and the relative phase velocity with the dimensionless wave number ωh and the Courant number Cr, corresponding to α=1 and different time-weightings, $\theta = 0, 0.5, 1.0$. It is evident that the Courant number and the time integration scheme have an influence on the numerical behavior of the MLS scheme for advection equation.

Expanding (10) and (11) in powers of ωh, we have

$$\zeta^h = 1+\frac{1}{2}Cr^2(1-2\alpha\theta)(\omega h)^2 - \frac{1}{24}Cr^2\left[2\alpha\theta+3Cr^2(1-4\alpha\theta(1-2\theta)-8\alpha^2\theta^3)\right](\omega h)^4 + O\left((\omega h)^6\right) \tag{12}$$

$$\frac{u^*}{u} = 1-\frac{1}{3}Cr^2[1-3\,\alpha\,\theta(1-\theta)](\omega h)^2 + \frac{1}{180}[-1+15\alpha Cr^2\theta(1-\theta) + 36Cr^4(1-5\alpha\theta(1-\theta)+5\alpha^2\theta^2(1-\theta)^2)](\omega h)^4 + O\left((\omega h)^6\right) \tag{13}$$

From (12) and (13), we note that the accuracy of ζ^h and u^*/u can reach at least 4^{th}-order in ωh, if α and θ satisfy the following criteria simultaneously:

$$\left\{ \begin{array}{l} 1-2\alpha\theta = 0 \\ 1-3\alpha\theta(1-\theta) = 0 \end{array} \right. \tag{14}$$

or alternatively

$$\begin{cases} \alpha = 3/2 \\ \theta = 1/3 \end{cases} \tag{15}$$

Figure 3 shows the variations in amplification factor ζ^h and relative phase velocity u^*/u of the MLS method corresponding to the values of α and θ defined by (15) as a function of ωh and Cr. We note from Figure 3 that when Cr =1, both the amplification factor and the relative phase velocity are equal to unity for all values of the dimensionless wave number ωh. Keeping Cr =1 and substituting (15) into (10) and (11) gives

$$\zeta^h\Big|_{\alpha=\frac{3}{2},\theta=\frac{1}{3},Cr=1} = 1 \tag{16a}$$

$$\frac{u^*}{u}\Bigg|_{\alpha=\frac{3}{2},\theta=\frac{1}{3},Cr=1} = 1 \tag{16b}$$

We should also note from (11) that $u^* = u$, even when Cr=1/2 and with the values of α and θ determined by (15); i.e.

$$\frac{u^*}{u}\Bigg|_{\alpha=\frac{3}{2},\theta=\frac{1}{3},Cr=\frac{1}{2}} = 1 \tag{17}$$

It follows from (16) that when Cr =1 and α and θ are determined by (15), there is no amplification and phase errors in MLS for all ωh, and all wave components included in the square wave will travel at the same speed giving rise to square wave without distortion. The MLS method with α and θ determined by (15) therefore can generate an accurate solution for the advection equation when Cr is kept at unity. This conclusion is confirmed by the numerical results presented in the ensuing section.

4 Numerical Analysis and Time-Adaptive Scheme

4.1 Advective Transport with Constant Flow Velocity

A one-dimensional advective transport problem involving a steep front with a constant flow velocity of u =0.5m/s, applicable to a region occupying [0, l] (where l=30m) is considered. The computational domain is discretized into 60 elements with a uniform elemental mesh of 0.5m. The initial concentration is zero everywhere in the domain, and the domain is subjected to boundary conditions $C|_{x=0} = 1$ and $\frac{\partial C}{\partial x}\Big|_{x=l} = 0$ at the left and the right boundaries of domain, respectively. Two time steps are chosen such that the Courant number is equal to 1/2 and 1, corresponding to the mesh size and flow velocity. Figure 4 illustrates the computational results for the normalized concentration as a function of the spatial and temporal coordinates obtained from the MLS scheme with the time-weighting and the upwind function defined by (15), and corresponding to two different Courant numbers; i.e. Cr=1/2 and Cr=1.0. From these results it is evident that the MLS scheme introduces oscillations in the vicinity of the discontinuity in the solution for Cr=1/2 , due to the deviation of the amplification factor from unity. The MLS scheme with α=3/2 and θ=1/3 can generate an accurate solution for the advection equation under the condition Cr=1.0 because of the criteria (16).

4.2 The Time-Adaptive Scheme

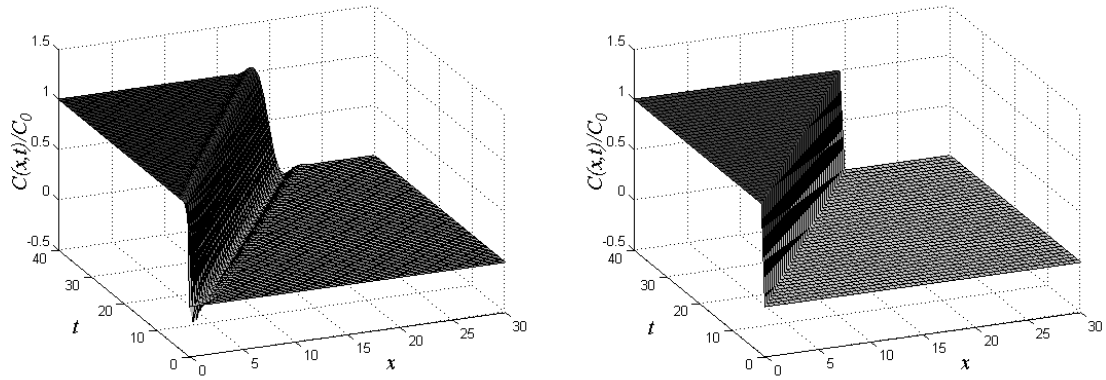
Since the Courant number has an important influence on the numerical performance of the MLS method, either a time-adaptive or a mesh-refining adaptive algorithm can be combined with the MLS method to obtain an accurate solution to the advective transport of a steep front in the presence of a transient flow velocity. In the adaptive scheme, either the time step Δt or size h_{ie} of the elements where a steep front is located should be determined on the basis of the magnitude of flow velocity, such that the Courant number satisfies

$$(Cr)_{ie} = \frac{|u|_{ie}\,\Delta t}{h_{ie}} = 1 \tag{18}$$

where ie indicates the elements that are located at the steep front and, h_{ie} and $|u|_{ie}$ are respectively the characteristic length and flow velocity of an element, N_{ie} is the total number of selected elements ie. Such a time-adaptive MLS method is used to simulate the advective transport process induced by a flow velocity with a time-dependency of the form

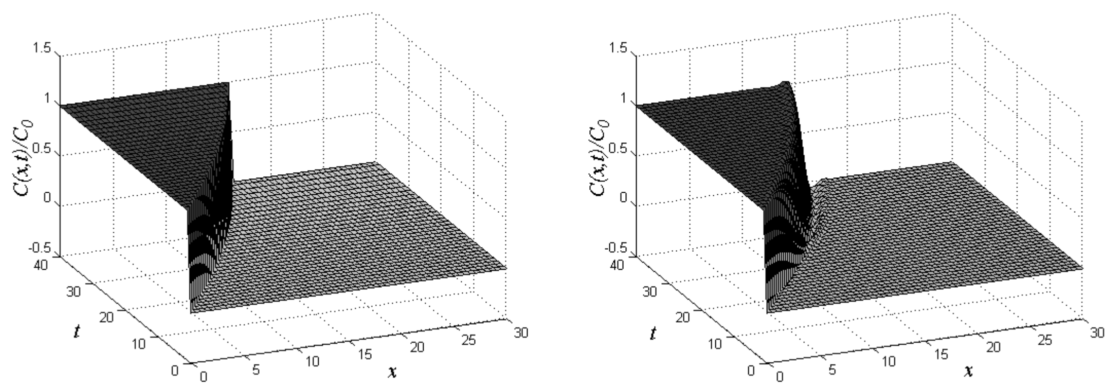
$$u = u_0 \exp(-\frac{k}{l}\,t) \tag{19}$$

where k is the Dupuit-Forchheimer hydraulic conductivity (which is related to the conventional area-averaged hydraulic conductivity $\tilde{k}$ by the relation $k = \tilde{k}/n^*$ and n^* is the porosity) and l is a length parameter corresponding to the size of the domain. Figure 5 shows the computational results for such an advective transport problem



(a) $\Delta t = 0.25$, $Cr = 0.5$ (b) $\Delta t = 0.5$, $Cr = 1.0$

Figure 4 : Computational results for the one-dimensional advective transport problem obtained from the MLS method with α=3/2 and θ =1/3.



(a) time-adaptive (b) non time-adaptive

Figure 5 : Computational results for the one-dimensional advective transport problem with an exponential decaying flow velocity obtained from the MLS method with α =3/2 and θ =1/3.

with k=0.03*m/day*, l=30m and u_0=0.5m/s obtained from the MLS method, both with and without a time-adaptive technique. The initial time step is taken as $\Delta t = 1.0s$, such that Cr=1 at the start of the transport process. With time, the flow velocity defined by (19) becomes smaller and the Courant number deviates from unity. With the time-adaptive scheme (18), which ensures that the elemental Courant number is always equal to unity during the computations, the MLS method generates a very accurate solution for the advective transport problem with the decaying flow velocity given by (19). Without a time-adaptive scheme, the MLS method gradually introduces oscillations in the vicinity of the discontinuity of the numerical solution, due to the deviation of the Courant number from the optimum value of unity.

5 Advective Transport in the Presence of a Hydraulic Transient

5.1 Governing Equation

In this section, we apply the time-adaptive scheme to the study of a one-dimensional advective transport problem related to a fluid-saturated porous medium. The advective flow velocity in the porous medium is governed by Darcy's law, which for an isotropic porous medium is given by

$$u = -k\frac{\partial \phi}{\partial x} \tag{20}$$

where k is the Dupuit-Forchheimer hydraulic conductivity, ϕ is the hydraulic potential inducing flow, which consists of the datum potential ϕ_D and the pressure potential ϕ_p, (i.e. $\phi = \phi_D + \phi_p$). Considering the compressibilities of the pore fluid and the porous skeleton and the mass conservation during flow, the partial differential equation governing the advective flow potential can be reduced to the following classical piezo-conduction equation for ϕ_p [Selvadurai (2000, 2002b)],

$$D_p \frac{\partial^2 \phi_p}{\partial x^2} = \frac{\partial \phi_p}{\partial t} \tag{21}$$

subject, respectively, to the boundary condition and the regularity condition

$$\phi_p(0,t) = \phi_0 \mathrm{H}(t); \quad \phi_p(\infty,t) \to 0 \tag{22}$$

as well as the initial condition

$$\phi_p(x,0) = 0; \quad x \in [0,\infty) \tag{23}$$

where $\mathrm{H}(t)$ is the Heaviside step function and ϕ_0 is a constant. We also note that, for the purposes of examining the pressure transients, the domain is assumed to be semi-infinite. This reduction is equivalent to assuming that the pressure head which initiates the flow is much larger than the datum head. The pressure diffusion coefficient D_p in (21) is given by

$$D_p = \frac{k}{S_s} = \frac{k}{\gamma_w [n^* C_f + C_s]} \tag{24}$$

where S_s is referred to as the storativity of the system, C_f is the compressibility of the pore fluid, and C_s is the compressibility of the porous skeleton.

Considering mass conservation of the chemical within a control volume, we obtain the following continuity equation for the advective transport process:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + C \frac{\partial u}{\partial x} = 0 \tag{25}$$

The third term on the LHS of (25) is non-zero if the fluid is considered to be compressible. It is evident that the governing PDEs (21) and (25) are weakly coupled, in the sense that the velocity field is assumed to be uninfluenced by the chemical transport process. The solution of the problem can be obtained in exact closed form through consideration of the appropriate solution applicable to the diffusion problem determined using a Laplace transform technique. The resulting solution takes the form

$$\phi_p(x,t) = \phi_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{D_p t}}\right) \tag{26}$$

where $\mathrm{erfc}(x)$ is the complimentary error function defined by

$$\mathrm{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-\zeta^2} d\zeta \tag{27}$$

Therefore, the velocity in the porous medium of semi-infinite extent is given by

$$u(x,t) = -k \frac{\partial \phi_p}{\partial x} = k\phi_0 \left(\frac{1}{\sqrt{\pi D_p t}} \exp\left(-\frac{x^2}{4D_p t}\right)\right) \tag{28}$$

Using (28) in (25) we obtain the following PDE governing the advective transport:

$$\frac{\partial C}{\partial t} + k\phi_0 \left(\frac{\exp\left(-\frac{x^2}{4D_p t}\right)}{\sqrt{\pi D_p t}} \right) \frac{\partial C}{\partial x} - k\phi_0 \left(\frac{x \exp\left(-\frac{x^2}{4D_p t}\right)}{2\sqrt{\pi}(D_p t)^{3/2}} \right) C = 0 \tag{29}$$

with the initial condition

$$C(x,0) = 0 \quad ; \quad x \in [0,\infty) \tag{30}$$

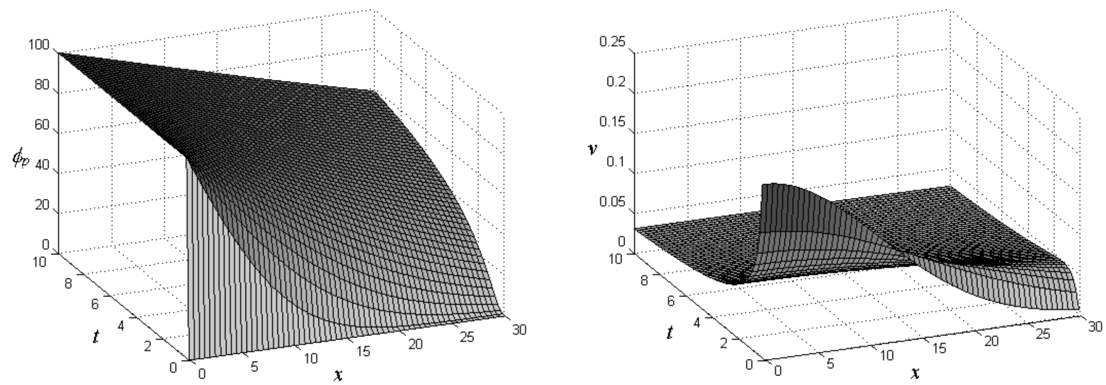
and subject to the boundary condition

$$C(0,t) = C_0 \mathrm{H}(t) \tag{31}$$

as well as the regularity condition

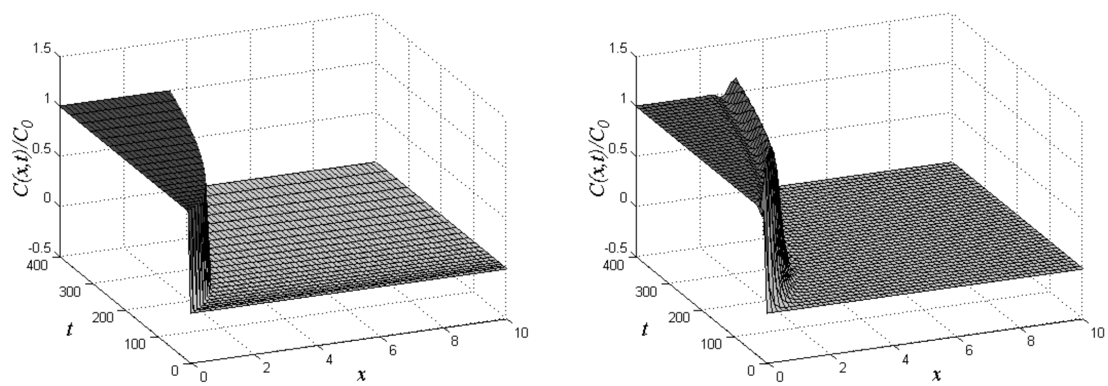
$$C(x,t) \to 0; \quad \text{as } x \to \infty \tag{32}$$

Therefore, for the flow process to be transient, the compressibility of the pore fluid and/or the compressibility of the porous skeleton should be non-zero. In the absence of these compressibilities, the flow process is governed by Laplace's equation with the consequence that for a mathematical solution to exist, the domain should be finite. In general the governing PDEs (21) and (25) are respectively parabolic and hyperbolic partial differential equations. The computational treatment of the hyperbolic PDE in particular is a non-routine exercise requiring special approaches that can address discontinuous fronts encountered during the transport of the chemical. The time-adaptive MLS scheme will be used to solve advective transport of a discontinuous front governed by (29).



(a) flow potential (b) flow velocity

Figure 6 : The time- and space-dependent distribution of (a) the flow potential and (b) the flow velocity .



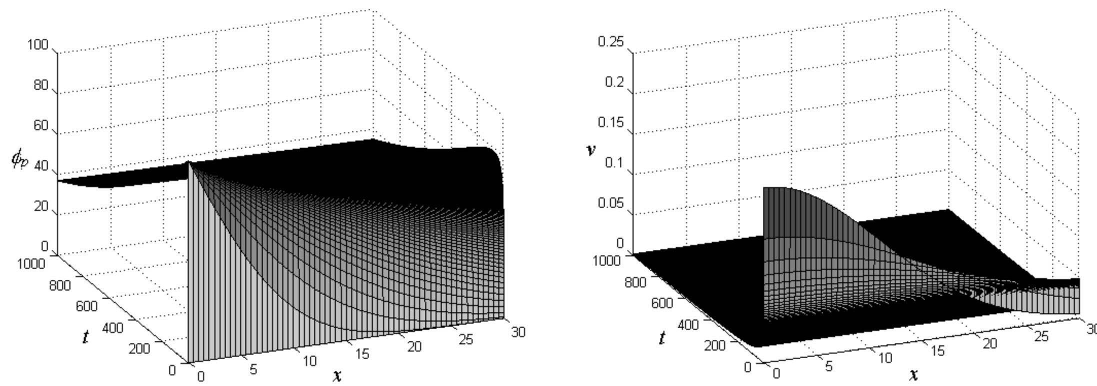
(a) time-adaptive (b) non time-adaptive

Figure 7 : Computational results for the advective transport in a porous medium with a transient advective flow velocity, obtained from the MLS method (t = 400 *days*), (a) with time-adaptive techniques (b) without time-adaptive techniques.

5.2 Numerical Computation

For the computations, we consider a finite region $\Omega=[0,l]$ with $l=30m$, which is subject to the boundary conditions of the flow potential $\phi(0)=\phi_0$ and $\phi(\infty)=0$, and the Dupuit-Forchheimer hydraulic conductivity for the porous medium is taken as $k=0.03m/day$. Typical values for the compressibilities for the porous aquifer material and the fluid are taken as $C_s=1.0\times10^{-8}m^2/N$ and $C_f=4.4\times10^{-8}m^2/N$ [Freeze and Cherry (1979)] respectively, and the porosity is taken as $n^*=0.3$. For these values, the specific storage parameter is approximately equal to $S_s=1.0\times10^{-8}m^2/N$.

First, we consider the case where the constant flow potential $\phi_0 = 100\,m$ is applied on the upstream boundary. Figure 6 shows the flow potential and flow velocity distribution during 0 to 10 days over the domain, which are obtained from analytical solutions (26) and (28) respectively. We note from Figure 6 that the flow velocity varies rapidly over the domain at the early stages of the transport due to the large variation in the potential and exhibits decay with time. The spatial domain Ω is discretized into 300 elements and the MLS method, both with and without the time-adaptive procedures is used to develop computational estimates for the advective transport problem. Figure 7 shows the corresponding numerical solutions obtained from the MLS method both with and without the time-adaptive scheme. Without the time-adaptive scheme, the MLS method will introduce oscillations in the solution due to the variation of the flow veloc-



(a) flow potential (b) flow velocity

Figure 8 : The space and time-dependent distribution of (a) the flow potential (b) the flow velocity corresponding to a decaying boundary potential.

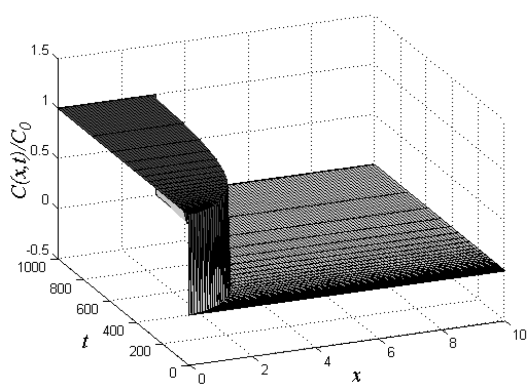


Figure 9 : Computational results for the advective transport in a porous medium with transient advective flow velocity obtained using a time-adaptive MLS method (t = 1000 *days*).

ity. The time-adaptive MLS method, however, gives an oscillation-free computational solution. With the time-adaptive scheme, the initial time step of Δt=0.2 *days* increases to Δt=33 *days* at the end of the computation to satisfy the constraint (18) imposed by the Courant number criterion.

We next consider a hydraulic pressure transient problem, where the boundary flow potential is assumed to decay as an exponential function of time

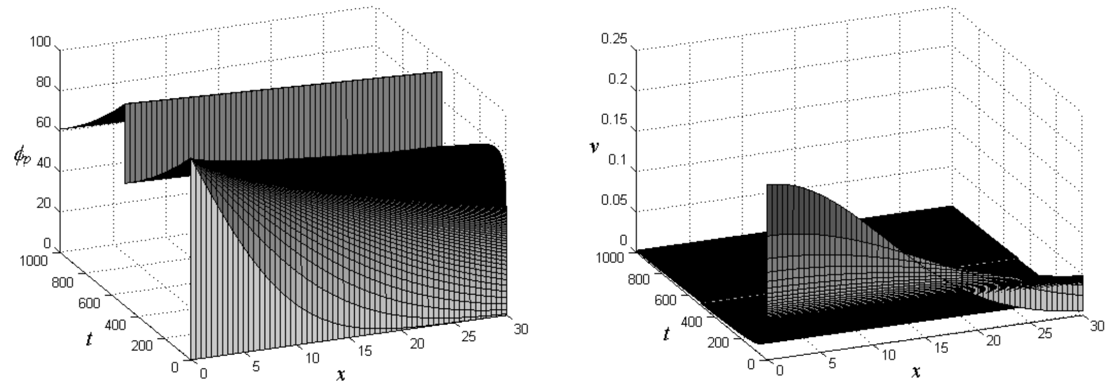
$$\phi_0 = \phi^* \exp(-\frac{k}{l}t) \tag{33}$$

where ϕ^*=100m. This potential variation can approximate the chemical entry under a gravity potential. Figure 8 illustrates the flow potential and velocity distribution over the domain during a 1000 *day* period. We note that the flow velocity decays almost to zero after 500 *days*. Figure 9 illustrates the numerical solution obtained from the time-adaptive MLS method which uses 100 elements. The initial time step of Δt=5 *days* increases to Δt=647*days* due to the low flow velocity at the location where the steep front of the solution is located, which implies that the chemical will migrate only 0.1m (element length) within 647*days*. We note from this figure that the advective transport process of the contaminant almost ceases due to the low flow velocity.

Finally, we apply the decaying boundary flow potential with a pulse as defined by the following time-dependent pressure history:

$$\phi_0 = \begin{cases} \phi^* \exp(-\frac{k}{l}t), & t \leq 500 \\ \\ \phi^* \exp[-\frac{k}{l}(t-500)], & t > 500 \end{cases} \tag{34}$$

Figure 10 illustrates the flow potential and velocity distribution over the domain up to a time duration of 1000 *days*. Figure 11 shows the corresponding numerical results, obtained using the time-adaptive MLS method with 100 elements. Again, with the adaptive scheme, the initial time step of Δt =5 *days* increases to Δt =142 *days* at the end of the simulation. We note from the numerical results shown in Figure 11 that the advective transport of the contaminant in the porous medium is accelerated at t=500 *days* due to the application of a pulse in the flow potential at the boundary.



(a) flow potential (b) flow velocity

Figure 10 : The time- and space-dependent distribution of (a) the flow potential and (b) the flow velocity corresponding to a time-dependent decaying boundary potential.

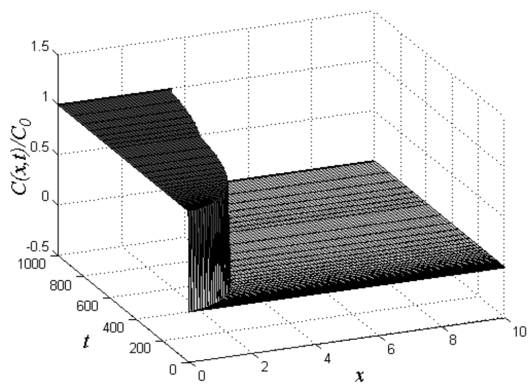


Figure 11 : MLS scheme-based computational results for the advective transport in a porous medium induced by a transient advective flow velocity; results applicable to a time-dependent decaying boundary potential (t = 1000 *days*).

6 Conclusions

A Fourier analysis shows that the time-marching scheme and the Courant number will have significant influences on the numerical performance of the Modified Least Squares method for the solution of the advective-transport equation. The upwind parameter introduced in the Modified Least Squares method and time weighting can be determined from a Fourier analysis conducted on the discretization of both the temporal and spatial terms of the advective-transport equation. It is shown from the Fourier analysis that the Modified Least Squares method with θ=1/3 and α=3/2 can generate oscillation-free solutions to the advective-transport equation when the Courant number is equal to unity. Based on this observation, a time-adaptive scheme is proposed to automatically select the time step in terms of the criterion Cr=1 for the advective transport problem with a transient flow velocity. Such a time-adaptive MLS method was used to simulate the advective transport of a chemical species with a profile that has a discontinuous front for a situation where the flow velocity is governed by a transient pressure field. Computational results show that the use of an MLS scheme with added features of a time-adaptive procedure results in an accurate method for the solution of the linear advection equation in the presence of a transient flow velocity.

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