INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 10, 623–636 (1990)

A LEAST-SQUARES PROCEDURE FOR THE SOLUTION OF TRANSPORT PROBLEMS

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SUMMARY

In this paper a least-squares formulation associated with a conjugate gradient algorithm is proposed for the solution of transport problems. In this procedure the advection–diffusion equation is first discretized in time using an implicit scheme. At each time step the resulting partial differential equation is replaced by an optimal control problem. This minimization problem involves the minimization of a functional defined via a state equation. This functional is chosen in order to force the numerical solution of the advection–diffusion equation to be equal to the hyperbolic advective part of this equation. The effectiveness of the method is shown through a one-dimensional example involving advective and diffusive transport. No oscillation and high accuracy have been obtained for the entire range of Peclet numbers with a Courant number well in excess of unity.

KEY WORDS Least-squares method Optimal control problem Conjugate gradient Advection–diffusion equation Perturbation series

1. INTRODUCTION

The purpose of this paper is to propose a new method for the numerical solution of advection–diffusion problems. This numerical method is based on a least-squares formulation of the advection–diffusion problem similar to the scaled least-squares method developed by Bristeaux *et al.*,[1] and consists of transforming a partial differential equation into an optimal control problem which is solved by a conjugate gradient algorithm and a finite element procedure.

Transport of pollutant in the atmosphere, lakes or rivers is commonly described by an advection–diffusion equation. The mathematical nature of this partial differential equation is commonly characterized by the dimensionless Peclet number

$$Pe = |\mathbf{v}| \frac{L}{\|\mathbf{D}_m\|}, \tag{1}$$

where $\mathbf{v}$ is the velocity vector, L is a characteristic length and $\|\mathbf{D}_m\|$ represents the Euclidean norm of the molecular diffusion tensor. When Pe is small, diffusion is dominant and the equation is closely parabolic. When Pe is large, advection dominates and the equation is closely hyperbolic.

When dealing with numerical solutions, the characteristic length is often taken as the size of the discretization, Δx. In addition to the numerical Peclet number, the numerical scheme may be affected by the relation between the time step and the size of the discretization, characterized by

0271–2091/90/060623–14$07.00

Received October 1988
Revised July 1989

the Courant number

$$\alpha_c = |v| \frac{\Delta t}{\Delta x}. \tag{2}$$

Numerical methods for solving an advection–diffusion problem may be classified into two groups: Eulerian methods, where the discretization in space is performed over a fixed grid in space, and Lagrangian methods, where the discretization is performed over a grid moving with the front.

Eulerian methods are efficient when dispersion is dominant and the distribution of concentration is relatively smooth. However, when the gradient of concentration of the pollutant is steep owing to the importance of advection (high Peclet number), these methods suffer from oscillations and large truncation errors.

Price *et al.*[2] pointed out the fact that oscillations are mainly due to spatial discretization. They proved that a central difference approximation will not oscillate provided

$$Pe\Delta x \leqslant 2. \tag{3}$$

Similar criteria to equation (3) have been proposed for weighted residual methods and for other finite difference schemes. However, these criteria are not always practical since they often require large computational time or large computer space.[3]

Upstream-weighting techniques have also been proposed for eliminating oscillations. In spite of the success of these types of methods for a large number of problems, they introduce large truncation errors which cause numerical dispersion.[4] The effect of this numerical dispersion is to smear the sharp front and therefore poor accuracy is obtained at high Peclet number. A large number of corrected finite difference schemes based on higher-order approximations in space have been proposed for reducing this numerical dispersion.[5]

High-order finite element techniques have also been proposed for the solution of advection–diffusion problems.[6] These methods are very efficient for a large number of problems; however, some of the numerical solutions proposed do not respect the mass balance.

It is important to note that in most of the Eulerian techniques proposed, numerical corrections have been done at a discretization level: element of a finite element procedure or point of a finite difference scheme. In the method proposed herein the correction term is formally introduced as a constraint defined on the whole space, independently of the finite element discretization.

In Lagrangian methods the advective terms are eliminated by a moving co-ordinate system. The resulting equation is a diffusion problem.[7,8] For high Peclet number, smooth solutions without oscillations and with good accuracy for various problems have been obtained by several authors.[7,8] However, techniques that involve a moving reference may be difficult to implement under particular conditions, e.g. complex boundary conditions, multiple-source terms or non-homogenous media.[9]

The high accuracy obtained by these methods, even for low Peclet number, is essentially due to the special numerical treatment near the front corresponding to the advective part of the equation.

Eulerian–Lagrangian methods combine the simplicity of a fixed Eulerian grid with the accuracy of the Lagrangian approach. The particle-tracking methods suggested by Garder *et al.*[10] are probably the most popular of the Eulerian–Lagrangian methods. In these methods the advection part of the problem is solved by the method of characteristics applied to a set of particles. The dispersion part of the problem is solved on a fixed grid by finite element or finite difference techniques. No oscillation and high accuracy have been obtained for a large number of problems. However, the results are very sensitive to the number of particles associated with each

element of the fixed grid and the implementation is made complicated by the presence of particles in the element of the fixed grid.

In our proposed method the advective part and the diffusive part of the transport equation are formally decoupled in a similar way to the Eulerian–Lagrangian scheme introduced by Neuman.[9] This separation is used for the mathematical definition of the objective function (or cost function) to minimize. For the advection–diffusion equation this objective function is proposed to be the sum of two terms: a first term corresponding to the parabolic behaviour of the equation and a constraint term corresponding to the hyperbolic behaviour of the equation at high Peclet number. In this paper the method is presented in a general form and computed on a one-dimensional example.

2. THEORY

2.1. Balance equation

The contaminant transport equation can be stated as

$$Rn\frac{\partial c}{\partial t}=\nabla\cdot(\mathbf{D}_h\nabla c+\mathbf{V}c)-R\lambda c+q \quad \text{in } \Omega, \tag{4}$$

where n ($[n]=L^3/L^3$) denotes the porosity of the porous medium, c ($[c]=M/L^3$) is the contaminant concentration, $\mathbf{D}_h$ ($[\mathbf{D}_h]=L^2/T$) is the hydrodynamic dispersion tensor, $\mathbf{V}$ ($[\mathbf{V}]=L/T$) is the fluid velocity, t is the time, q is a source or sink term, λ is used to represent the processes of reaction or decay of contaminants in the porous medium and R is the retardation factor.

The hydrodynamic dispersion tensor $\mathbf{D}_h$ can be expressed as[11]

$$\mathbf{D}_h=\left((\alpha_L-\alpha_T)\frac{\mathbf{V}\mathbf{V}^T}{\|\mathbf{V}\|}+\alpha_T\|\mathbf{V}\|\mathbf{I}\right)+\mathbf{D}^*, \tag{5}$$

where α_T and α_L denote the longitudinal and transverse dispersivities respectively, $\|\mathbf{z}\|$ denotes the Euclidean norm of the vector $\mathbf{z}$, $\mathbf{I}$ is the unit matrix and $\mathbf{D}^*$ is the molecular diffusion coefficient.

2.2. Initial and boundary conditions

The initial conditions are given by

$$c(\mathbf{x},0)=c_0(\mathbf{x}), \tag{6}$$

where $\mathbf{x}$ is the position vector and c_0 is a known function.

The boundary conditions can be stated in a general form as

$$(-\mathbf{D}_h\nabla c+\mathbf{V}c)\cdot\mathbf{n}+\alpha_i(c-C)=Q \quad \text{on } \Gamma_i, \tag{7}$$

where $\mathbf{n}$ is the unit outward normal vector along the boundary Γ_i, C and Q are prescribed functions of space and time, and α_i determines the nature of the boundary condition acting on Γ_i. The condition along the boundary can vary from prescribed flux ($\alpha_i = 0$) to prescribed concentration ($\alpha_i = \infty$). For intermediate values of α_i the condition is mixed.

2.3. Advection–Diffusion equation for large Peclet number

The numerical difficulties appearing in the Eulerian scheme for large Peclet number are due to the advective nature of the equation. In the following a perturbation method is used to analyse

the mathematical behaviour of the advection–diffusion equation for large values of the Peclet number.

A non-dimensional form of the above advection–diffusion equation may be obtained by introducing the following non-dimensional parameters:

$$\phi(x) = \frac{c}{c_{\text{ref}}}, \tag{8}$$

where c_{ref} corresponds to a constant reference concentration value;

$$\bar{\nabla} = \frac{\nabla}{\Delta x}$$

for the non-dimensional nabla operator;

$$\mathbf{D} = \frac{\mathbf{D}_h}{\|\mathbf{D}_h\|}$$

for the non-dimensional dispersion tensor;

$$\mathbf{u} = \frac{\mathbf{V}}{|\mathbf{V}|}$$

for the non-dimensional fluid velocity.

The non dimensional form of the advection–diffusion equation can be written as

$$Rn \frac{\partial \phi}{\partial \tau} = \bar{\nabla} \cdot \left(\frac{\mathbf{D}}{Pe} \bar{\nabla} \phi + \mathbf{u}\phi \right) - \frac{R\lambda \Delta x \phi}{|\mathbf{V}|} + \frac{q \Delta x}{c_{\text{ref}} |\mathbf{V}|} \quad \text{in } \Omega, \tag{9}$$

where $\tau = t|\mathbf{V}|/\Delta x$.

The corresponding initial and boundary conditions are given by

$$\phi(\mathbf{x}, 0) = \frac{c_0(\mathbf{x})}{c_{\text{ref}}}, \tag{10}$$

$$\left[\left(-\frac{\mathbf{D}}{Pe} \bar{\nabla} \phi + \mathbf{u}\phi \right) \right] \cdot \mathbf{n} + \frac{\alpha_i}{|\mathbf{V}|} \left(\phi - \frac{C}{c_{\text{ref}}} \right) = \frac{Q}{|\mathbf{V}| c_{\text{ref}}} \quad \text{on } \Gamma_i. \tag{11}$$

The behaviour of the solution of the above non-dimensional equation may be studied by expanding ϕ in a perturbation series in $1/Pe$,

$$\phi(x) = \phi_0(x) + \sum_{i=1}^{\infty} \frac{\phi_i(x)}{(Pe)^i}, \tag{12}$$

where ϕ_0 is the solution of the hyperbolic equation

$$Rn \frac{\partial \phi_0}{\partial \tau} = \bar{\nabla} \cdot (\mathbf{u}\phi_0) + \frac{R\lambda \Delta x \phi_0}{|\mathbf{V}|} + \frac{q \Delta x}{c_{\text{ref}} |\mathbf{V}|} \quad \text{in } \Omega, \tag{13}$$

$$\phi_0(\mathbf{x}, 0) = \frac{c_0(\mathbf{x})}{c_{\text{ref}}}, \tag{14}$$

$$\mathbf{u}\phi_0 \cdot \mathbf{n} + \frac{\alpha_i}{|\mathbf{V}|} \left(\phi_0 - \frac{C}{c_{\text{ref}}} \right) = \frac{Q}{|\mathbf{V}| c_{\text{ref}}} \quad \text{on } \Gamma_i \tag{15}$$

and ϕ_1 is the solution of a hyperbolic equation containing a known diffusion term on the right-hand side:

$$Rn\frac{\partial \phi_1}{\partial \tau} = \bar{\nabla}\cdot(\mathbf{u}\phi_1) + \bar{\nabla}\cdot(\mathbf{D}\bar{\nabla}\phi_0) \quad \text{in } \Omega, \tag{16}$$

$$\phi_1(\mathbf{x}, 0) = 0, \tag{17}$$

$$(-\mathbf{D}\bar{\nabla}\phi_0 + \mathbf{u}\phi_1)\cdot\mathbf{n} + \frac{\alpha_i}{|\mathbf{V}|}\phi_1 = 0 \quad \Gamma_i. \tag{18}$$

For any n, ϕ_n is the solution of the following hyperbolic equation:

$$\frac{\partial \phi_n}{\partial \tau} = \bar{\nabla}\cdot(\mathbf{u}\phi_n) + \bar{\nabla}\cdot(\mathbf{D}\bar{\nabla}\phi_{n-1}) \quad \text{in } \Omega, \tag{19}$$

$$\phi_n(\mathbf{x}, 0) = 0, \tag{20}$$

$$(-\mathbf{D}\bar{\nabla}\phi_{n-1} + \mathbf{u}\phi_n)\cdot\mathbf{n} + \frac{\alpha_i}{|\mathbf{V}|}\phi_n = 0 \quad \text{on } \Gamma_i. \tag{21}$$

Analytical solution of the hyperbolic equations governing ϕ_n can be found using the method of characteristics.[7, 12]

Note that ϕ_0 defines the equation of the front of the advection–diffusion equation. It corresponds to a limiting case of infinite Peclet number. For large Peclet numbers the solution of ϕ_n is concentrated near the front; therefore far from the front the solution of the advection–diffusion equation will be nearly equal to ϕ_0.

A mathematical algorithm for solving the advection–diffusion equation has to take into account the limiting mathematical behaviour. For the consideration of this problem one can impose that the numerical solution be equal to ϕ_0 except on a domain moving with the front.

Another type of constraint is to impose that for large Peclet number the numerical scheme be equal to the perturbation expansion (equation (12)).

These two types of constraint will be introduced in the least-squares procedure presented in the next section.

3. LEAST-SQUARES FORMULATION OF THE PROBLEM

We first discretize in time the advection–diffusion equation (equation (4)) using either an explicit or implicit scheme. The implicit discretization chosen for the transport equation may be written as follows.

For the initial condition,

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}). \tag{22}$$

After l iterations in time,

$$Rn\beta(c^{l+1} - c^l) = \nabla\cdot(\mathbf{D}_h\nabla c^{l+1} - \mathbf{V}c^{l+1}) - R\lambda c^{l+1} + q \quad \text{in } \Omega. \tag{23}$$

The corresponding boundary conditions are given by

$$(-\mathbf{D}_h\nabla c^{l+1} + \mathbf{V}c^{l+1})\cdot\mathbf{n} + \alpha_i(c^{l+1} - C) = Q \quad \text{on } \Gamma_i, \tag{24}$$

where $\beta = 1/\Delta t^l$ and Δt^l represents the time step after l iterations in time. For simplification of the formulation, C will be taken equal to zero in the further development.

In the present algorithm the discretized partial differential equation (equation (23)) is formulated in terms of an optimal control problem.

3.1. Optimal control problem

A possible least-squares formulation of equation (23) may be written as

$$\min_{(\xi \in V_g)} J(\xi(c^{l+1})) = \frac{1}{2}\int_\Omega \beta \|\xi\|^2 + \|\nabla\xi\|^2 \, d\Omega, \tag{25}$$

where $\xi(c^{l+1})$ is an auxiliary function, called the state vector, dependent on the solution c^{l+1} through the state equation.

A strong formulation of this equation may be written as: find $\xi \in V_g$ such that

$$\beta\xi - \Delta\xi = Rn\beta(c^l - c^{l+1}) + \nabla\cdot(\mathbf{D}_h\nabla c^{l+1} - \mathbf{V}c^{l+1}) - R\lambda c^{l+1} + q \quad \text{in } \Omega, \tag{26}$$

subject to the boundary conditions

$$\nabla\xi\cdot\mathbf{n} = 0 \quad \text{on } \Gamma_q, \tag{27}$$

where Γ_q corresponds to mixed and von Neumann boundary conditions (α_q finite). V_g is the Sobolev functional space associated with the state equation:

$$V_g = \{\xi \in H^1(\Omega);\ \xi|_{\gamma_p} = 0\}, \tag{28}$$

where

$$H^1(\Omega) = \{\xi \in L^2(\Omega);\ (\partial\xi/\partial x_i) \in L^2(\Omega),\ i = 1, 2, 3\} \tag{29}$$

and γ_p corresponds to zero Dirichlet boundary conditions ($\alpha_p = \infty$, $C = 0$).

Before going further in the development of the method, one has to ensure that the solution of the optimal control problem is the solution of the discretized advection–diffusion problem.

By virtue of the Green theorem, the cost function $J(\xi(c^{l+1}))$ can be written as

$$J(\xi(c^{l+1})) = \frac{1}{2}\left(\int_\Omega (\beta\xi - \Delta\xi)\xi \, d\Omega + \int_\Gamma (\nabla\xi\cdot\mathbf{n})\xi \, d\Gamma\right) \tag{30}$$

where Γ represents the union of all the boundaries Γ_i. Inserting the boundary conditions of the state equation into the mathematical expression of $J(\xi(c^{l+1}))$, one can get

$$J(\xi(c^{l+1})) = \frac{1}{2}\left(\int_\Omega [Rn\beta(c^l - c^{l+1}) + \nabla\cdot(\mathbf{D}_h\nabla c^{l+1} - \mathbf{V}c^{l+1}) - R\lambda c^{l+1} + q]\xi \, d\Omega\right). \tag{31}$$

$J(\xi(c^{l+1}))$ is a positive function and therefore its minimum value will be zero. The last expression of $J(\xi(c^{l+1}))$ shows clearly that c^{l+1} is also the solution of the optimal control problem.

Note that this result is due to the choices of the boundary conditions of the state equation and the Sobolev space V_g. If we want to introduce Dirichlet boundary conditions of the type $c = C$, the present least-squares formulation is not adopted. Another choice of cost function, state equation and Sobolev space has to be made.

The state equation may also be written in a weak form, used in a Galerkin finite element procedure: find $\xi \in V_g$ such that for $\nabla\psi \in V_g$,

$$\int_\Omega (\beta\xi\psi + \nabla\xi\cdot\nabla\psi)d\Omega = \int_\Omega Rn\beta(c^l - c^{l+1})\psi + (\mathbf{D}_h\nabla c^{l+1} - \mathbf{V}c^{l+1})\cdot\nabla\psi$$
$$- R\lambda c^{l+1}\psi + q\psi \, d\Omega - \int_{\Gamma_q} [(\mathbf{V}\cdot\mathbf{n} + \alpha_q)c^{l+1} - Q]\psi \, d\Gamma. \tag{32}$$

The optimal control problem is solved by a conjugate gradient algorithm.

3.2. Conjugate gradient algorithm

Let $J'(\xi(c^{l+1}))$ denote the gradient of the cost function (equation (25)) and (ψ, w) the scalar product associated with the cost function.

For $\psi \in V_g$ and $w \in V_g$,

$$(\psi, w) = \int_\Omega (\beta\psi w + \nabla\psi \cdot \nabla w)\, d\Omega. \tag{33}$$

Then the different steps of a conjugate gradient algorithm applied to the solution of equation (25) are described as follows.

Step 0

$$c_0^{l+1} \in V_g.$$

Compute $g^0 \in V_g$ such that for all $\psi \in V_g$,

$$(\psi, g^0) = -\langle J'(\xi(c_0^{l+1})), \psi \rangle \tag{34}$$

and

$$z_0 = -g^0. \tag{35}$$

Computation of the (n+1)th iteration. c_n^{l+1}, g^n and the search direction z_n are known functions.

Step 1: Descent. Find

$$\lambda^n = \operatorname{argmin} J(\xi(c_n^{l+1} + \lambda z_n)), \quad \lambda \in \mathbb{R} \tag{36}$$

(line search),

$$c_{n+1}^{l+1} = c_n^{l+1} + \lambda^n z_n. \tag{37}$$

Step 2: New descent direction. Compute $g^{n+1} \in V_g$ such that for all $\psi \in V_g$,

$$(\psi, g^{n+1}) = -\langle J'(\xi(c_{n+1}^{l+1})), \psi \rangle \tag{38}$$

and

$$z_{n+1} = -g^{n+1} + \gamma^{n+1} z_n. \tag{39}$$

In the classic version of the algorithm γ^{n+1} is taken as

$$\gamma^{n+1} = \frac{(g^n, g^n)}{(g^{n-1}, g^{n-1})}. \tag{40}$$

In the present work the Nazareth version[13] of the Conjugate Gradient Algorithm was implemented.

Each evaluation of $J(\xi(c^{l+1}))$ for a given argument c^{l+1} requires the solution of the state equation (26) in order to obtain the vector ξ.

The calculation of ξ_{j+1} from c_{j+1}^{l+1} in the conjugate gradient algorithm requires also the solution of a similar elliptic problem. This second problem requires the mathematical calculation of $J'(\xi(c^{l+1}))$. The gradient of the cost function $J(\xi)$ may be formally defined as:[1] for all $\mathbf{w} \in V_g$,

$$\langle J'(\xi(c^{l+1})), \mathbf{w} \rangle = \lim \frac{J(\xi(c^{l+1} + t\mathbf{w})) - J(\xi(c^{l+1}))}{t}, \tag{41}$$

$$t \to 0, \qquad t \neq 0. \tag{42}$$

A formal expression of $J'(\xi)$ may be obtained directly from the weak formulation of the state equation (26). The details of this algebraic development are presented in the Appendix, where it is shown that $\langle J'(\xi(c^{l+1})), \psi \rangle$ can be identified with the linear functional

$$\mathbf{w} \to \int_\Omega (Rn\beta \mathbf{w}\xi + \mathbf{D}_h \nabla \mathbf{w} \cdot \nabla \xi + \mathbf{w}\mathbf{V} \cdot \nabla \xi - R\lambda \xi)\, d\Omega. \tag{43}$$

Therefore a weak formulation of equations (34) and (37) may be written as: find $\eta \in V_g$ such that for all $\mathbf{w} \in V_g$,

$$\int_\Omega (\beta \eta \mathbf{w} + \nabla \eta \cdot \nabla \mathbf{w})\, d\Omega = \int_\Omega (Rn\beta \mathbf{w}\eta + \mathbf{D}_h \nabla \mathbf{w} \cdot \nabla \eta + \mathbf{w}\mathbf{V} \cdot \nabla \eta - R\lambda \eta)\, d\Omega. \tag{44}$$

3.3. Objective function for advection–diffusion problem

The choice of the objective function is not unique; it depends on the choice of the functional space V_g on which the minimization is done. The mathematical form of the objective function corresponds to a norm associated with the functional space V_g. For quick convergence this chosen norm has to be appropriate to the state equation.[1]

The objective function presented above (equation (26)) is not appropriate for the solution of transport problems, especially for high Peclet number. This is due to the fact that the state equation has the structure of a diffusion problem.

Numerical tests performed with the present formulation did not give satisfactory results. Results similar to upstream-weighting techniques have been obtained. Smearing near the front, small oscillations and numerical dispersion appear at high Peclet number.

With the present cost function, the proposed algorithm belongs to the Eulerian-type methods and does not take into account the hyperbolic aspect of the problem. At high Peclet number the solution of the advection–diffusion problem is very close to the associated hyperbolic advective equation $\bar{c} = c_{ref}\phi_0$ (see Section 2). Moreover, these two solutions will be nearly equal except on a domain near the front.

In order to consider this mathematical behaviour, one can impose that the solution and its gradient be equal respectively to the advective solution $\bar{c}$ and its gradient outside this domain moving with the front. This is done by introducing an integral constraint in the cost function. A first possible choice for the corrected cost function is

$$J_1(\xi(c^{l+1})) = \frac{1}{2}\int_\Omega \beta \|\xi\|^2 + \|\nabla \xi\|^2\, d\Omega + \mu(Pe) \int_{\Omega - D^\varepsilon_{l+1}} |c^{l+1} - \bar{c}^{l+1}|^2 + |\nabla(c^{l+1} - \bar{c}^{l+1})|^2\, d\Omega, \tag{45}$$

where $\bar{c}^{l+1} = c_{ref}\phi(x, t^{l+1})$ and D^ε_{l+1} defines the moving domain after l iterations in time:

$$D^\varepsilon_{l+1} = \{\mathbf{x} \in \Omega; |(c^{l+1} - \bar{c}^{l+1})| \geqslant \varepsilon\}, \tag{46}$$

where ε represents a small positive number. $\mu(Pe)$ is the Lagrangian coefficient representing the relative weight of the constraint in the minimization procedure.

A rigorous method for the determination of $\mu(Pe)$ is a difficult mathematical task. However, $\mu(Pe)$ is adjusted in order to reinforce the constraint for high Peclet number and to neglect it for small Peclet number.

One can argue that a rigorous determination of D^ε_{l+1} at each time step can be difficult, especially for complicated problems. Moreover, the computation of the constraint integral over

$\Omega - D_{l+1}^{\varepsilon}$ using a finite element procedure requires the selection of nodal points and elements inside D_{l+1}^{ε} at each time step. Therefore, for difficult problems involving mixed boundary conditions or source terms, the implementation of the method may be complicated.

This problem is similar to the determination of the 'zone of computation' appearing in Lagrangian methods.[7, 8] For simple problems of constant velocity, the moving co-ordinate system method can be used for a rigorous determination of D_{l+1}^{ε}.

A way of overcoming the difficulty of the moving domain is to introduce a more restrictive constraint. We could force the solution to be equal to the perturbation series, presented in Section 2, for large Peclet numbers. The corresponding cost function may be written as

$$J_2(\xi(c^{l+1})) = \frac{1}{2}\int_{\Omega} \beta \|\xi\|^2 + \|\nabla\xi\|^2 \, d\Omega + \mu(Pe)\int_{\Omega} |c^{l+1} - \bar{c}_{n_0}^{l+1}| + |\nabla(c^{l+1} - \bar{c}_{n_0}^{l+1})| \, d\Omega, \tag{47}$$

where

$$\bar{c}_{n_0}^{l+1} = c_{\text{ref}}\left(\phi_0(x) + \sum_{i=1}^{n_0} \frac{\phi_i(x)}{(Pe)^i}\right). \tag{48}$$

This second formulation involve the analytical or numerical determination of each ϕ_i, $i = 1, \ldots, n_0$.

From a mathematical point of view, in both cases, the addition of constraints does not require a change of the functional space V_g. It is easily shown that these new cost functions define two new norms on V_g. It is not yet clear how good the choice of norm and state equation is from a convergence point of view.

Although the second approach is of interest, it will not be pursued in the present work. In the following section a one-dimensional example is presented with the least-squares moving domain formulation (16).

4. EXAMPLE

The governing transport equation may be written as

$$D\frac{\partial^2 c}{\partial^2 x} - V\frac{\partial c}{\partial x} = n\frac{\partial c}{\partial t}. \tag{49}$$

4.1. Problem I

The initial and boundary conditions relative to Problem I are

$$c(0, 0) = c_0, \tag{50}$$

$$c(x, 0) = 0, \quad x \geqslant 0, \tag{51}$$

$$\frac{\partial c}{\partial x}(0, t) = 0, \tag{52}$$

$$c(\infty, t) = 0. \tag{53}$$

The least-squares formulation of Problem I is written

$$\min_{(\xi \in V_g)} J_1(\xi(c^{l+1})), \tag{54}$$

where $\xi(c^{l+1})$ is the solution of the state equation (26) and the Sobolev space V_1:

$$V_1 = \{\psi \in H^1((0, 1)); \psi(1) = 0\}. \tag{55}$$

The moving domain is determined using a moving co-ordinate system. For $\varepsilon = 0{\cdot}01$ it can be shown that the diffusion length L is[7]

$$L = 3{\cdot}6/\sqrt{(Pe)}. \tag{56}$$

For the computation $D_{l+1}^{0{\cdot}01}$ was defined as a segment of length L and centre Vt^l.

A linear dependence with respect to Pe was assumed for $\mu(Pe)$:

$$\mu(Pe) = Pe, \qquad Pe \leqslant 100, \tag{57}$$

$$\mu(Pe) = 100, \qquad Pe \geqslant 100. \tag{58}$$

Table I. Values of physical parameters for Problem I

Parameter	Value	Pe	Figure
Darcy velocity V	1 m day^{-1}		
Porosity n	0·25		
Molecular diffusion coefficient D_0	0·01 m^2 day^{-1}		
Longitudinal dispersivity α_L for case 1	5 m	2	1
Longitudinal dispersivity α_L for case 2	2 m	5	2
Longitudinal dispersivity α_L for case 3	0·2 m	50	3
Longitudinal dispersivity α_L for case 4	0·0 m	$+\infty$	4
Concentration at the source, c_0	1 mg m^{-3}		

$\Delta x = 10$ m; $\Delta t = 2{\cdot}5$ days.

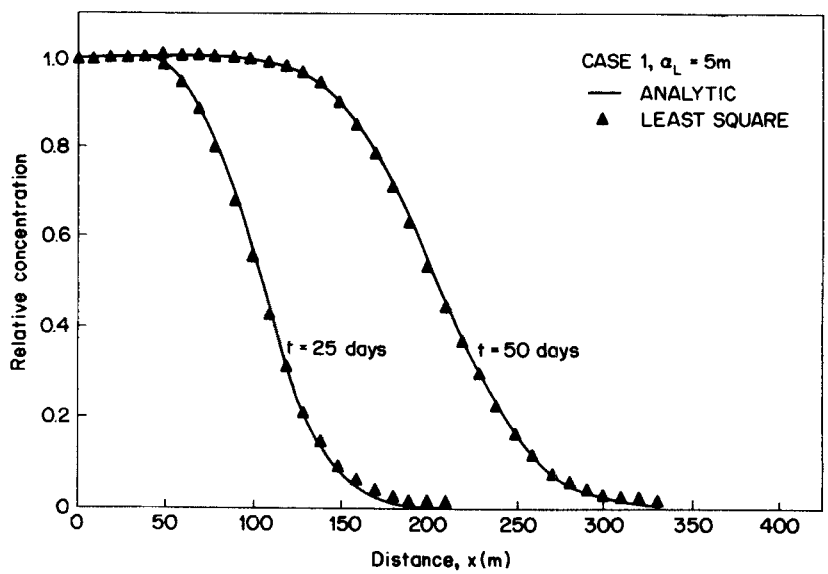

Figure 1. Comparison of analytical and numerical solutions for Problem I, case 1

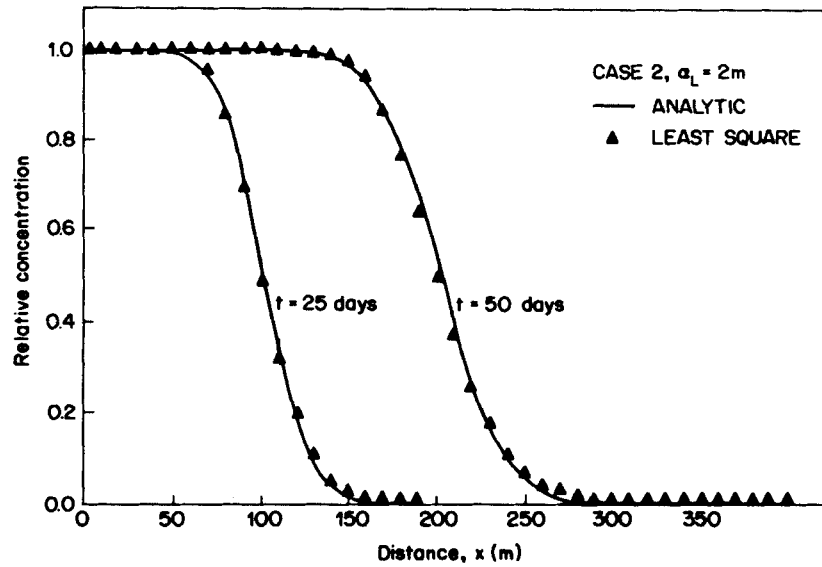

Figure 2. Comparison of analytical and numerical solutions for Problem I, case 2

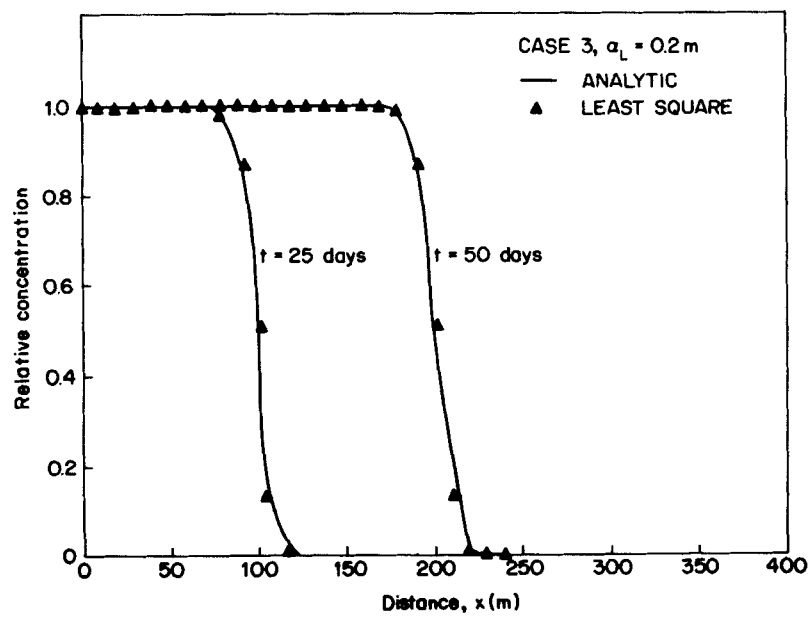

Figure 3. Comparison of analytical and numerical solutions for Problem I, case 3

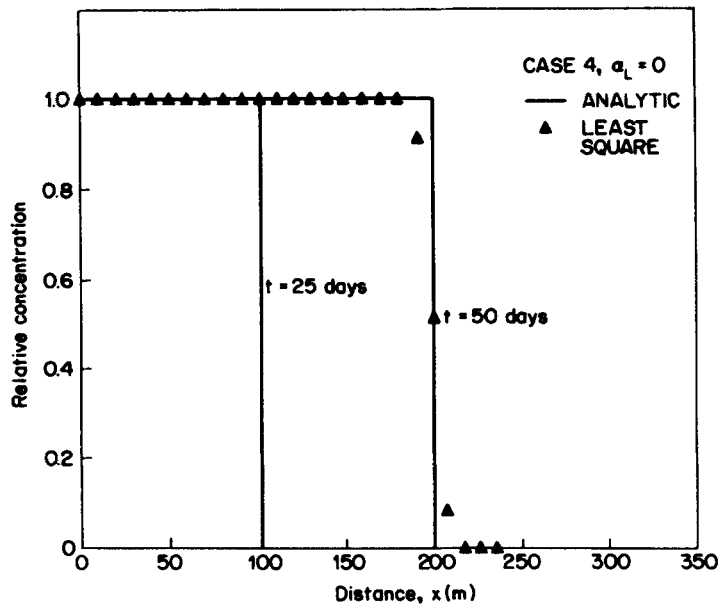

Figure 4. Comparison of analytical and numerical solutions for Problem I, case 4

The numerical procedure was compared with the analytical solution found in Reference 11:

$$\frac{c}{c_0} = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{nx - Vt}{2(Dt)^{1/2}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{nx + Vt}{2(Dt)^{1/2}}\right)\right]. \tag{59}$$

With the notation of Section 2, the diffusivity D may be written as

$$D = \alpha_L V + D^*. \tag{60}$$

The grid chosen for the finite element procedure comprises 10 elements of equal size $\Delta x = 10$ m.

Four values of Peclet number were considered, corresponding to different longitudinal dispersivity α_L. A list of the values of the physical parameters is given on Table I.

In Figures 1–4 the results of the computation are presented for a time step $\Delta t = 2{\cdot}5$ days.

At low Peclet number (cases 1 and 2) the results are similar to those of the Galerkin finite element code existing in the literature.[14] However, for large Peclet number (cases 3 and 4) no oscillation appears and high accuracy has been obtained.

Case 3 ($Pe = 50$) was tested for different time steps $\Delta t = 0{\cdot}25$, 1, $2{\cdot}5$ and 5 days. A difference of 2%–5% between the different solutions was obtained.

5. CONCLUSIONS

A general least-squares formulation for the solution of transport problems has been presented. The novel feature of the method resides in the choice of a suitable functional which takes into account the parabolic nature of the problem for low Peclet number and its hyperbolic nature for large Peclet number.

The method has been employed to solve a one-dimensional problem. The numerical results obtained demonstrate the high accuracy of the present method and the absence of oscillation and

numerical diffusion. In spite of the Eulerian co-ordinates used, the results seem to be nearly independent of the Courant number.

Further investigations of the method in the future will include numerical improvements such as acceleration of the algorithm, and analysis of one-, two- and three-dimensional problems with different types of boundary conditions.

APPENDIX: CALCULATION OF THE GRADIENT OF THE COST FUNCTION

The direct computation of $J'(\xi(c^{l+1}))$ from the definition of the gradient, equation (25), requires the computation of $\xi(c^{l+1} + t\mathbf{w})$.

From the weak formulation of the state equation, one can get: for all $\psi \in V_g$,

$$\begin{aligned}\int_\Omega (\beta\xi\eta + \nabla\xi\cdot\nabla\psi)\,d\Omega = \int_\Omega [&Rn\beta(c^l - c^{l+1})\psi + (\mathbf{D}_h\nabla c^{l+1} - \mathbf{V}c^{l+1})\cdot\nabla\psi \\ &- R\lambda c^{l+1}\psi + q\psi]\,d\Omega \\ &- \int_{\Gamma_q} [(\mathbf{V}\cdot\mathbf{n} + \alpha_q)c^{l+1} - Q]\psi\,d\Gamma \\ &+ t\left(\int_\Omega (Rn\mathbf{w}\psi + \mathbf{D}_h\nabla\mathbf{w}\cdot\nabla\psi + \mathbf{w}\mathbf{V}\cdot\nabla\psi - R\lambda w)\,d\Omega\right). \end{aligned} \tag{61}$$

The above expression suggests that

$$\xi(c^{l+1} + tw) = \xi(c^{l+1}) + t\eta, \tag{62}$$

where η is the solution of: for all $\psi \in V_g$,

$$\int_\Omega (\beta\eta\psi + \nabla\eta\cdot\nabla\psi)\,d\Omega = \int_\Omega (Rn\beta\mathbf{w}\psi + \mathbf{D}_h\nabla\mathbf{w}\cdot\nabla\psi + \mathbf{w}\mathbf{V}\cdot\nabla\psi - R\lambda w)\,d\Omega. \tag{63}$$

We are now able to express the cost function at the point $\xi(c^{l+1} + tw)$. From equation (25) one can get

$$J(\xi(c^{l+1} + tw)) = J(\xi(c^{l+1})) + t\int_\Omega (\beta\eta\xi + \nabla\eta\cdot\nabla\xi)\,d\Omega + O(t^2). \tag{64}$$

Therefore from the definition of the derivative and from equation (63) one can get

$$\langle J'(\xi(c^{l+1})), \psi\rangle = \int_\Omega (Rn\beta\mathbf{w}\xi + \mathbf{D}_h\nabla\mathbf{w}\cdot\nabla\xi + \mathbf{w}\cdot\nabla\xi - R\lambda w)\,d\Omega. \tag{65}$$

The same calculation can be performed for the computation of $J_1'(\xi(c^{l+1}))$; it is easily shown that

$$\begin{aligned}\langle J_1'(\xi(c^{l+1})), \psi\rangle = &\int_\Omega (Rn\beta\mathbf{w}\xi + \mathbf{D}_h\nabla\mathbf{w}\cdot\nabla\xi + \mathbf{w}\mathbf{V}\cdot\nabla\xi - R\lambda w)\,d\Omega \\ &+ \mu(Pe)\int_{\Omega - D_{i+1}^c} (c^{l+1}w + \nabla c^{l+1}\cdot\nabla w)\,d\Omega. \end{aligned} \tag{66}$$

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