MATHEMATICS DEPARTMENT

Application of the Taylor-Galerkin Method to Transport Problems in Subsurface Hydrology

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Numerical Analysis Report 5/93

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A model for saline intrusion - an example of non-passive, non-reactive, single-species contaminant transport in a porous medium - is presented. A computational algorithm for approximating the solution of this contaminant transport model is given.

An implicit Taylor-Galerkin method is used to discretise the contaminant continuity equation (which takes the form of an advection-diffusion equation). This discretisation method gives a non-symmetric matrix system (due to the fully implicit treatment of the advection term) which is solved by the Bi-CGSTAB non-

ontents

This report is concerned with the numerical modelling of non-passive, non-reactive, single-species contaminant transport in saturated porous media. In this type of flow, a contaminant is carried through a porous medium by a fluid; the contaminant does not undergo any chemical or biological reactions but its presence does affect the physical properties of the fluid, e.g. density, viscosity.

A common example of this type of flow is saline intrusion - saltwater moving inland and mixing with less dense freshwater. In regions where coastal aquifers are utilised for water supply, saline intrusion leads to a degradation of groundwater quality. To control this, an accurate and reliable model for the shape and position of the saltwater front is required to predict the response to changes in usage patterns. A solution of this type of problem is the object of this work.

There is a transition zone between the freshwater and the saltwater caused by hydrodynamic dispersion. In some circumstances, the width of this zone is small relative to the thickness of the aquifer so that it may be approximated as a sharp interface [1]. This report is concerned with flows in which the sharp interface approximation is not valid and a full variable density model must be used.

Variable density transport models are well documentedctiont;i));y tre

ef throeeTbffw;;6tmanXT

io Tre fluid;T)1bqfi6flensitX)fiq)6yX1ffq;6,XTb1)wfi6flnXT))bqfi6flgeneralXT)fibq)6btXT)1bqfi6f

In non-passive contaminant transport, the presence of the contaminant affects the properties of the fluid; it is assumed that only the density of the fluid is affected in this work. The contaminants considered are non-reactive so there are no chemical effects to consider. A mathematical model which governs flows of this type in porous media can be formulated in terms of

1. a continuity equation for the fluid,
2. a continuity equation for the contaminant, and

—

-3

-2

$=$

-1

2

$=$

$-1 \quad -1$

In this work, it is assumed that is constant and equal to the viscosity of the non-contaminated fluid, $_0$. Hence the fluid flux equation can be written in terms of the piezometric head as

$$= \; \underline{\underline{\;}} \quad + (\quad) \frac{}{} \tag{1}$$

where $\underline{\underline{\;}} = \frac{\underline{\underline{\mathbf{k}}}\rho g}{\mu_0}$ is the hydraulic conductivity tensor (LT^{-1}). From [1], in the absence of source terms the fluid mass balance equation for saturated flow (i.e. flow in which the moisture content is equal to the porosity and hence independent of time) is

$$\frac{}{} + \quad (\quad) = 0 \tag{2}$$

where is the porosity of the porous medium. Substitution of from (1) into (2) constitutes the fluid continuity equation.

From [1], in the absence of source terms the contaminant mass balance equation for saturated flow is

$$\frac{(\quad)}{} + \qquad \underline{\underline{\;}} (\quad) = 0 \tag{3}$$

where $\underline{\underline{\;}} = \underline{\underline{\;}}(\quad)$ is the dispersion tensor (L^{2}T^{-1}). The ( ) entry in the disper-

[illegible]

()

$$ij \qquad T \qquad m \quad ij \qquad L \qquad T \frac{i \;\; j}{}$$

T

L

m

ij

$2 \quad -1$

A Taylor-Galerkin method for the advection-diffusion equation was given in Donea

$$\frac{\quad}{\quad} \quad \frac{\quad}{\quad} \quad \frac{{}^2}{{}^2}$$

$$\frac{\quad}{\quad} \quad \frac{{}^2}{\quad}\frac{{}^2}{{}^2} \quad {}^3$$

$$\frac{{}^2}{{}^2} \quad \frac{\quad}{\quad} \frac{\quad}{\quad}$$

$$\frac{\quad}{\quad} \quad \frac{{}^2}{{}^2} \quad \frac{\quad}{\quad} \quad \frac{{}^2}{{}^2}$$

$$2\frac{{}^2}{{}^2} \quad \frac{{}^3}{{}^3} \quad 2\frac{{}^4}{{}^4}$$

$$\frac{\ ^2}{\ ^2}(\quad + \Delta \ ) \quad \frac{1}{\Delta} \quad —(\quad + \Delta \ ) \quad —(\quad)$$

so that the Taylor series becomes

$$(\quad) = \ (\quad + \Delta \ ) \quad \frac{\Delta}{2} \quad —(\quad + \Delta \ ) + —(\quad) \ + \mathrm{O}(\Delta \ )^3 \qquad (8)$$

It is interesting to note that the Taylor-Galerkin formulation used here for the advection-diffusion equation leads to a standard Crank-Nicolson temporal discretisation. Using (7) to replace the temporal derivatives by spatial ones gives $\ ^2$

$$\frac{\quad}{\quad} \qquad - \quad \frac{}{} \qquad \frac{}{}$$

$$- \quad \frac{\ ^2}{\ ^2} \qquad \frac{\ ^2}{\ ^2}$$

$$\sum_{j}^{nodes} \frac{}{} \ _j \qquad _j \qquad _i \ _j$$

$$\sum_{j}^{nodes} \ _j \qquad _j \quad - \quad _i \frac{\ _j}{} \quad - \quad _i \frac{\ ^2 \ _j}{\ ^2}$$

$$\frac{}{} \quad ^2 \frac{\ ^4}{\ ^4} \quad \frac{}{} \quad ^2 \frac{\ ^3}{\ ^3}$$

Although this leads to a symmetric system, it has the stability restriction of the explicit Taylor-Galerkin method.

In the remainder of this report, the un-split implicit Taylor-Galerkin method for the advection-diffusion equation given by (9) is used in the solution of problems involving transport of non-reactive, single-species contaminants in saturated porous media.

4 Numerical Solution of the Governing Equations

In this section, the methods used to discretise and solve the governing equations from Section 2 are described.

4.1 Partial Coupling

Owing to the dependency of the fluid density, ρ, on the contaminant concentration, c, in the constitutive equation (4), the fluid mass and contaminant mass balance equations are coupled (and the contaminant mass balance equation is non-linear).

In order to solve such a problem, the mass balance equations must either be solved simultaneously with a non-linear iteration (which doubles the order of the problem) or an iteration must be performed between them at each time step, with a non-linear iteration performed on the contaminant mass balance equation during each coupling iteration.

However, in the types of problems considered in this report, the coupling is of a relatively weak nature (i.e. $\frac{\partial \rho}{\partial c}$ is small). Hence, for transient computations, a "partially coupled" approach is adopted in which the term that causes the coupling (the density) is treated explicitly. This linearises the contaminant mass balance equation and also allows the two mass balance equations to be solved separately during each time step [7], dramatically decreasing the complexity and computational cost.

With this partially coupled approach, the structure of each time step is

1. The fluid density at this time step is approximated explicitly by linear extrapolation of the densities from the two previous time steps, i.e.

$$\rho^{n+1} \approx \rho^n + \frac{(\Delta t)^{n+1}}{(\Delta t)^n}(\rho^n - \rho^{n-1}).$$

2. The fluid continuity equation ((1)   (2)) is solved for the piezometric head.

3. The Darcy velocity field is calculated using the fluid flux equation (1).

4. The contaminant mass balance equation (3) is solved for the contaminant concentration.

$$= \quad = \quad \Gamma \quad {}^{h}_{n}$$

$$= \quad \Gamma \quad {}^{h}_{n}$$

method to give

$$= ^{n+1}(\quad \Phi^{n+1} + \quad ^{n+1} \quad) \ \Omega + \quad \frac{}{\Delta}(\quad ^{n+1} \quad ^{n}) \ \Omega = {}_{\Gamma} \quad ^{n+1} \ {}^{h,n+1}_{n} \ \Gamma$$

where the superscripts denote the discrete time level. This weak form is then

$$I$$

$$\sum_{J=1}^{nodes} \quad {}_J \quad {}_J$$

$$J$$

$$J$$

$$^{n+1} \qquad \frac{}{} \quad ^{n+1} \qquad ^{n}$$

$$_{IJ} \ {}_{I,J=1,\ldots,nodes} \qquad {}_I \ {}_{I=1,\ldots,nodes}$$

$$^{n+1} \qquad {}^{n+1}_{J} \ {}_{J=1,\ldots,nodes} \qquad ^{i} \qquad {}^{i}_{I} \ {}_{I=1,\ldots,nodes}$$

$$_{IJ} \quad {}_e \quad {}^{e}_{IJ} \quad {}_e \quad {}_e \quad {}_I = {}^{n+1} \quad {}_J \quad {}^{e}$$

$$_{I} \quad {}_e \quad {}^{e}_{I} \quad {}_e \quad {}^{n+1} \quad {}^{h}_{n} \ {}^{n+1} \quad \Gamma^{e} \quad {}_I \quad {}^{e} \quad {}^{n+1} \quad {}_e \quad {}_I = {}^{n+1} \quad {}^{e}$$

$$^{i}_{I} \quad {}_e \quad {}^{e,i}_{I} \quad {}_e \quad {}^{i} \quad {}_e \quad {}_I \quad {}^{e}$$

is symmetic and positive definite if the tensor $\underline{\underline{\ }}^{n+1}$ is symmetric and positive definite ([4], p212). For a reasonably fine spatial discretisation, the system is also large and sparse so an iterative solution method is preferable. A suitable solution technique is the incomplete Cholesky preconditioned conjugate gradient method (ICCG) [11] which is used in this work.

An average value of the Darcy velocity of the fluid on each element, which is needed in the contaminant mass balance part of the model, is calculated using the fluid flux equation (1).

xpressed in terms of the transformed variable, Φ, which is calculated in the solution of the fluid continuity equation, the fluid flux equation is

$$= \underline{\underline{\ }} \frac{\Phi}{\ } +$$

This equation is discretised by the standard Galerkin finite element method. Treating the material and fluid properties in the same manner as for the fluid continuity equation then leads to the matrix system

$$\sum_{J=1}^{nodes} {}^{n+1}_{e} \quad {}_{e} \quad {}_{I} \quad {}_{J} \; \Omega^e = \sum_{J=1}^{nodes} \Phi_J^{n+1} \; {}_{e} \; \frac{\underline{\underline{\ }}}{{}^{n+1}} \; {}_{e} \quad {}_{I} \quad {}_{J} \; \Omega^e$$

$$ {}_{e} \underline{\underline{\ }}^{n+1} \quad {}_{e} \quad {}_{I} \; \Omega^e$$

$$(\; = 1 \; 2 \; \ldots \;)$$

The matrix in this systemΩ

$^{n+1}$

4.4 Contaminant Mass Balance Equation

Substituting (2) into (3) leads to the following form of the contaminant mass balance equation,

$$\rho\phi\frac{\partial c}{\partial t} + (\rho\mathbf{q}).\nabla c = \nabla.\left\{\phi\underline{\underline{\mathbf{D}}}\nabla(\rho c)\right\}. \tag{10}$$

This is an advection-diffusion equation, which is discretised by the implicit Taylor-Galerkin method outlined in Section 3 by using (10) to replace the temporal derivatives in an approximate Taylor series expansion of the form (8), and then performing a spatial discretisation by the standard Galerkin finite element method.

This leads to the following matrix system which is the fully discretised form of the contaminant mass balance equation

$$\left\{\frac{1}{\Delta t}A + \frac{1}{2}\left(B^{n+1} + C^{n+1}\right)\right\}\mathbf{c}^{n+1} = \left\{\frac{1}{\Delta t}A - \frac{1}{2}\left(B^{n} + C^{n}\right)\right\}\mathbf{c}^{n} - \frac{1}{2}(\mathbf{F}^{n+1} + \mathbf{F}^{n}),$$

where

$$\begin{array}{ll} A = \{A^i_{IJ}\}_{I,J=1,\ldots,nodes} & \\ B^i = \{B^i_{IJ}\}_{I,J=1,\ldots,nodes} & \mathbf{c}^i = \{c^i_J\}_{J=1,\ldots,nodes} \\ C^i = \{C^i_{IJ}\}_{I,J=1,\ldots,nodes} & \mathbf{F}^i = \{F^i_I\}_{I=1,\ldots,nodes}, \end{array}$$

and

$$\begin{aligned} A_{IJ} &= \sum_e A^e_{IJ} = \sum_e \int_e N_I N_J d\Omega^e \\ B^i_{IJ} &= \sum_e B^{e,i}_{IJ} = \sum_e \int_e \nabla N_I.\langle\underline{\underline{\mathbf{D}}}\rangle^i \nabla N_J d\Omega^e \\ C^i_{IJ} &= \sum_e C^{e,i}_{IJ} = \sum_e \frac{\langle\mathbf{q}\rangle^i}{\langle\phi\rangle}.\int_e N_I \nabla N_J d\Omega^e \\ F^i_I &= \sum_e F^{e,i}_I = \sum_e \frac{\langle q^c_n\rangle^i}{\langle\rho\rangle^i\langle\phi\rangle}\int_{\Gamma^e} N_I d\Gamma^e. \end{aligned}$$

The angled brackets have the same meaning as in the discretisation of the fluid continuity equation.

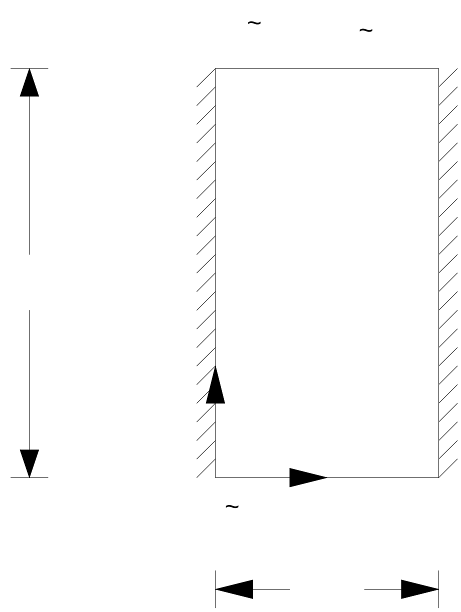
The matrix in this system has three components, the mass matrix A which is symmetric and positive definite, the stiffness matrix B^{n+1} which is symmetric and positive definite (with the same assumptions on the structure of $\underline{\underline{\ }}^{n+1}$ as for $\underline{\underline{\ }}^{n+1}$ in Section 4.2) and the advection matrix $^{n+1}$ which is non-symmetric and indefinite. Hence the system is non-symmetric and, as with the discrete fluid

^{2} ^{2} $^{-8}$

$-$

xx xz zx zz -4

L T m



x z -5

The Courant and mesh Peclet numbers for this problem are

$$= \frac{{}_z \Delta}{\Delta} \qquad\qquad = \frac{\Delta}{L}$$

where Δ is the time step and Δ is the vertical mesh size.

Initially, the concentration of the tracer is zero everywhere inside the region. The tracer front moves down the column under the action of gravity and this front disperses as it moves. Until the tracer reaches the bottom of the column, this problem can be analysed as one on a semi-infinite domain in which the boundary conditions are,

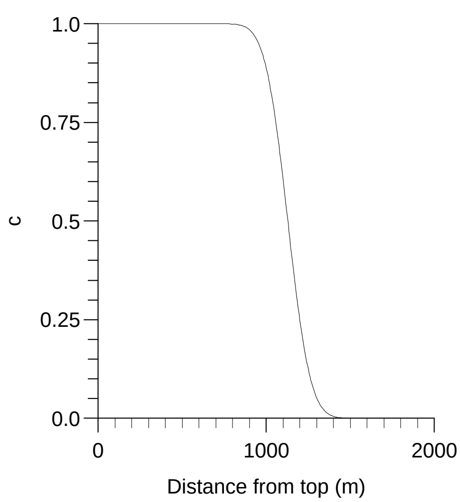
$$\begin{aligned} \tilde{}(\quad 2000 \quad) &= 1 \\ \tilde{}(\qquad\qquad) &= 0 \\ {}^{c}_{n}(0 \qquad) &= 0 \\ {}^{c}_{n}(10 \qquad) &= 0 \end{aligned}$$

The analytic solution to this problem has been derived in [12] as

$$(\qquad) = \frac{1}{2} \; \exp \; \frac{{}_z(2000 \qquad)}{zz} \; \mathrm{erfc} \; \frac{2000 \qquad\quad {}_z}{2 \; \overline{\quad zz}} \; + \mathrm{erfc} \; \frac{2000 \qquad + \; {}_z}{2 \; \overline{\quad zz}}$$

z

$$\overline{\quad} = \int_s^{\infty} \; {}^{-u^2}$$


1.0
0.75
0.5
0.25
0.0
c
0
1000
2000
Distance from top (m)

is almost a discontinuity. To reduce the oscillations this may cause, for the case with $= 5$, the time step is started from $\Delta \;\; = 5 \quad 10^4$ s. (corresponding to $= 0\ 5$) and increased by a factor of 1.2 at each time step to a maximum value of $\Delta \;\; = 5 \quad 10^5$ s. (corresponding to $= 5$).

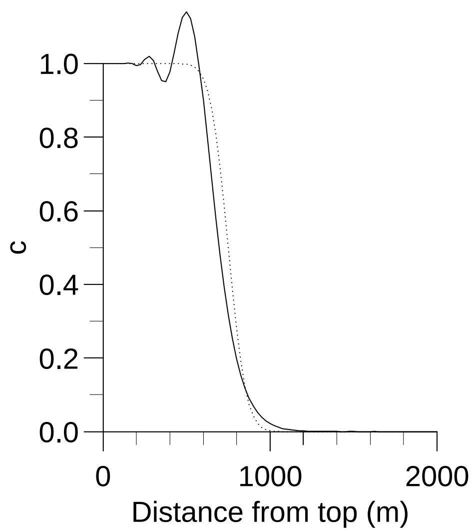
$$\text{i.e. } (\Delta \;\;)_{new} = \min(1\ 2 \quad (\Delta \;\;)_{old}\ 5 \quad 10^5 \text{ s.})$$

From Table 1, for $= 0\ 5\ \ 1$ the solution is monotone, but for $= 5$ oscillations in the solution cause un-physical extrema to be created (the maximum value of the dimensionless concentration is greater than one).

Non-physical concentrations can be disastrous in reactive transport models where they affect the chemical terms. Flux-corrected transport methods [2, 19] - i.e. local averaging of the scheme with a positive[1] lower order scheme - may be used in these cases to control the oscillations. However, as this report is not concerned with reactive transport, oscillations are regarded as acceptable as long

	6			
	7			
	7			
	6			
	7			
	7			
	6			
	7			
	7			

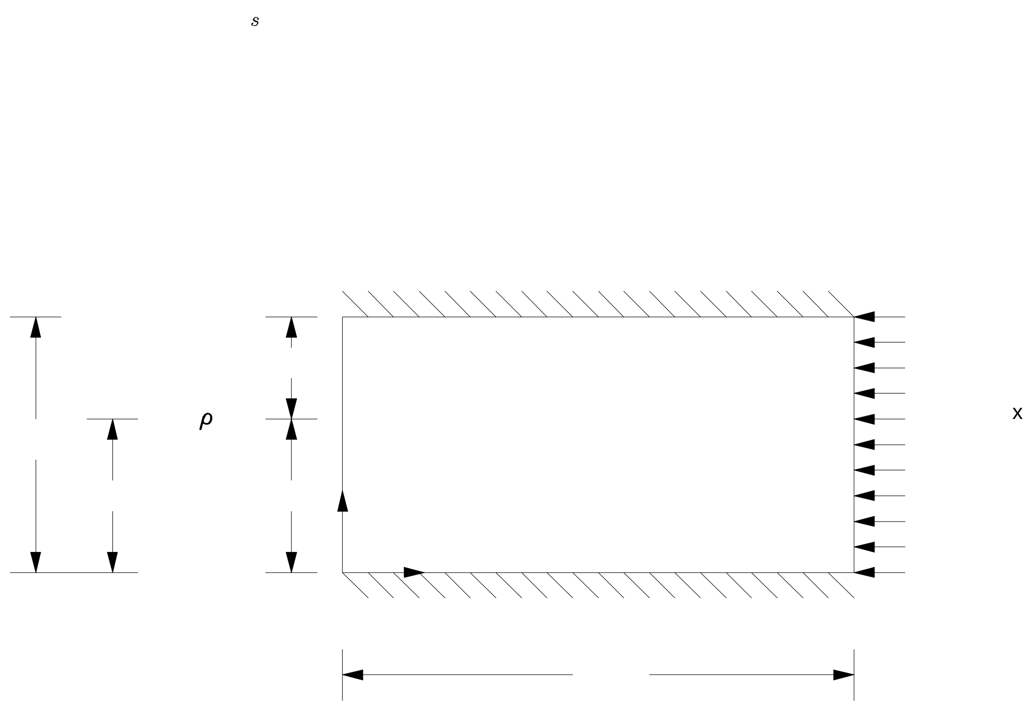
[1]Positivity is the multidimensional generalisation of monotonicity.



1.0
0.8
0.6
0.4
0.2
0.0
c
0
1000
2000
Distance from top (m)

The Henry problem [8] is a 2-D, saturated, groundwater flow problem which involves fresh-water in a confined aquifer discharging to a vertical open sea boundary over a diffuse wedge of sea-water that has intruded into the aquifer. An approximate analytic solution to the Henry problem was given in the original paper but no known numerical model matches this solution.

In [17] it is suggested that there may be an inaccuracy in the approximate analytic solution caused by missing higher-order terms which were originally dis-



consists of two components as shown in Figure 6. On the lower part of the coastal boundary (0 $_1$) the dimensionless salt concentration is set to unity, while on the remainder of the coastal boundary ($_1$ 1m) the prescribed dispersive solute mass flux, $\frac{c}{n}$, is set to zero.

Now $_1$ is not known but there are two ways of determining this value. In the first (used in e.g. [9]), an initial guess for $_1$ is made and a solution

1

1

1

x 1

x 1

x

1

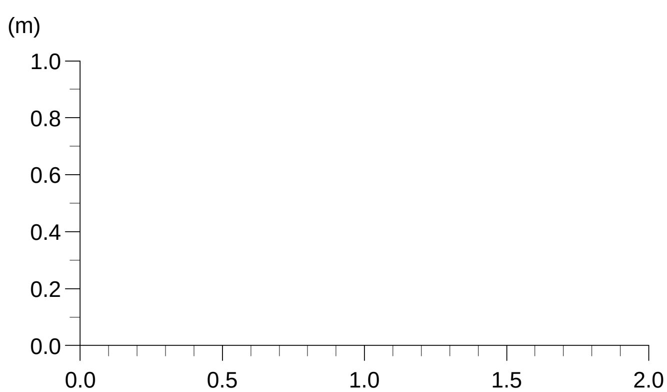
1

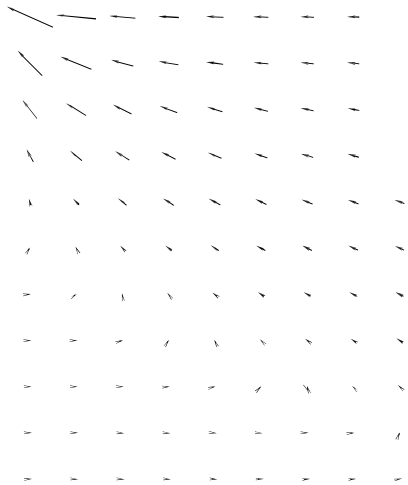
2 0

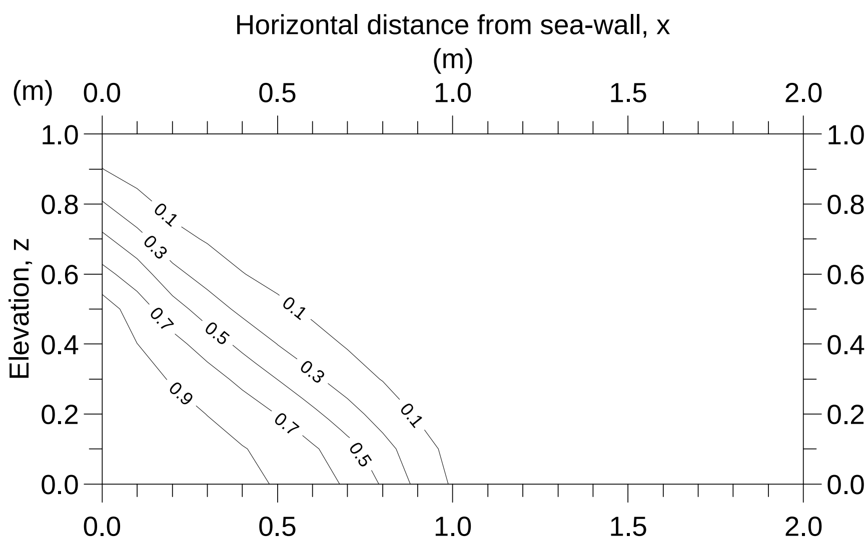
0 3 $\frac{\partial \rho}{\partial c}$ 3

= = −9 2 =

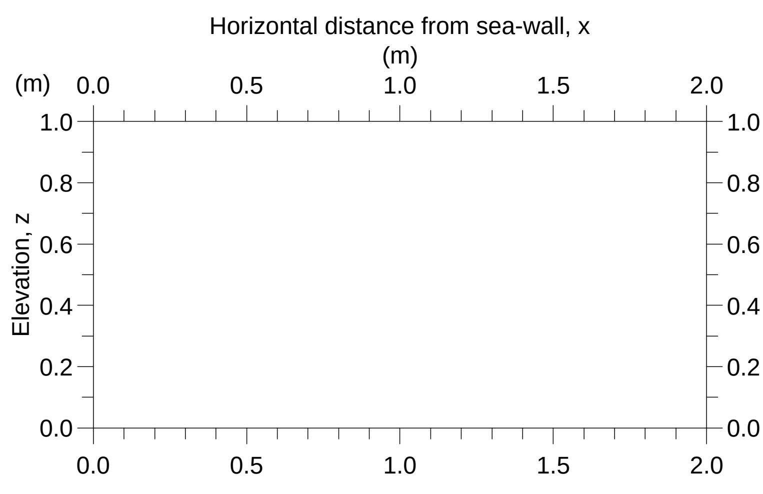
L T m −6 2


(m)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.5
1.0
1.5
2.0





Horizontal distance from sea-wall, x
(m)
(m)
0.0
0.5
1.0
1.5
2.0
Elevation, z
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.3
0.5
0.7
0.9


Horizontal distance from sea-wall, x
(m)
(m)
0.0
0.5
1.0
1.5
2.0
Elevation, z
1.0
0.8
0.6
0.4
0.2
0.0

6 oncluding Remarks

The variable density model for contaminant transport in porous media with a Taylor-Galerkin discretisation for the contaminant continuity equation gives transient results which agree well with analytical solutions and with those from the literature.

The partially coupled approach, in which the weak dependence of the fluid density on the contaminant concentration is exploited by treating the term which causes the coupling between the fluid and contaminant continuity equations (the density) explicitly, is valid for the problems encountered in transient saline intrusion modelling. This approach leads to a substantial decrease in the computational cost.

The fully implicit Taylor-Galerkin method with linear basis functions is equivalent to the Crank-Nicolson finite element method. Although this discretisation method is demonstrated for problems on two-dimensional regular grids in this report, it is fully multi-dimensional and operates on irregular grids in the same way.

For the test cases presented, the diagonally preconditioned Bi-CGSTAB solver converges in an acceptable number of iterations (e.g. $< \sqrt{n}$, where n is the order of the matrix). However, as the Courant number is increased, the advection part of the global matrix (i.e. the component which causes the non-symmetry) becomes more dominant, which may lead to a degradation in the performance of the Bi-CGSTAB solver. The performance of the non-symmetric solver has not been investigated in this report, this aspect of the solution method is the subject of a future study.

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