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Numerical modeling of coupled hydrological phenomena using the Modified Eulerian–Lagrangian method

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ABSTRACT

The chapter presents the advantages of using the Modified Eulerian–Lagrangian (MEL) method for solving the transport of extensive quantities in a porous medium. In this modified formulation, the material derivatives are written in terms of modified velocities. These are the velocities at which the various phase and component variables propagate in the domain, along their respective characteristic curves. It is shown that these velocities depend on the heterogeneity of various solid matrix and fluid properties. Accordingly, an extension to the Peclet number is presented that also accounts for governing equations that may be advective dominant with no reference to the fluid velocity or even when this velocity is not introduced.

A mathematical analysis proves that for coupled partial differential equations (PDEs), unlike the Eulerian implicit finite difference scheme the MEL method unconditionally guarantees the absent of spurious oscillations.

The MEL formulation is demonstrated for a coupled set of PDEs concerning the problem of saltwater intrusion, with heat transfer.

A numerical example suggests that the MEL scheme produces better resolution compared to the Eulerian and the Eulerian-Lagrangian ones.

INTRODUCTION

The numerical solution of the solute transport equation introduces difficulties mainly because of certain terms that may conform this equation to become hyperbolic dominant. Such cases may be when the advective flux or when the gradient of the dispersion factor become predominate. The numerical solution of such cases may result in problems of numerical dispersion and over/under shooting errors.

The Eulerian-Lagrangian (EL) methods have been developed as special techniques for solving the advection dominated transport problems. All EL schemes are based on the advection part solved along characteristic pathlines. An EL least-square collocation method was proposed by Bentley and Pinder (1992). The EL collocation method with the use of the method of characteristics for the advective problem was documented by Baptista (1987) and by Allen and Khosravani (1990). The performance of the EL methods and sources of errors in such schemes were discussed by Bentley and Pinder (1992).

Neuman (1981, 1984), Neuman and Sorek (1982), Sorek and Braester (1988), and Sorek (1985a, 1985b, 1988) also decompose the dependent variable into advective and residual parts. The resulting advection problem is solved by tracking particles along pathlines and the dispersive problem is solved on a fixed grid.

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None of these solutions incorporate the gradient of the dispersion factor as part of the velocity that drives the particle along its pathline.

Following the formulation of the MEL method (Bear et al., (1997) and its mathematical analysis (Sorek et al., 1998), the MEL formulation here is exemplified for the flow, the solute transport, and the heat-transfer equations referring to hydrodynamic processes in porous media. These PDEs are coupled when considering, e.g., the saltwater-intrusion problem. In the case of the MEL formulation for the flow equation, particle velocity is associated with the gradient of the hydraulic conductivity while, e.g., for the transport equation it also accounts for the gradient of the hydrodynamic dispersion. The numerical scheme is based on the decomposition of the differential operator and the dependent variables.

THEORY

General case

Consider the transport of an extensive quantity, E, of a fluid phase occupying part of the void space of a porous medium domain. Let S and e denote the saturation of the phase and the density of E within it, respectively.

The macroscopic Eulerian balance equation of E of a phase, within a porous medium domain, can be written in the form

$$\frac{\partial}{\partial t}(\phi S e) = -\nabla \cdot [\phi S(e\mathbf{V} - \mathbf{D}_h^E \cdot \nabla e)] - f_{\alpha\to\beta}^E + \phi S \rho \Gamma^E, \tag{1}$$

where ϕ denotes the porosity, $\mathbf{V}$ denotes the mass weighted velocity of the phase, $f_{\alpha\to\beta}^E$ denotes the transfer of E from the considered α phase to all other (β) phases across common (microscopic) interphase boundaries, ρ denotes the mass density of the phase, and Γ^E denotes the rate of growth (source) of E per unit mass of the phase. We often combine $\mathbf{J}^{*E}$, the dispersive flux of E (due to variations in e and in $\mathbf{V}$ at the microscopic level) and $\mathbf{J}^E$, the diffusive flux of E (relative to the mass averaged velocity), by introducing the hydrodynamic dispersive flux $\mathbf{J}_h^E$ $(= \mathbf{J}^{*E} + \mathbf{J}^E)$. Let us also assume that the flux of hydrodynamic dispersion of E can be expressed as a Fickian-type expression, i.e.,

$$\mathbf{J}_h^{*E} = -\mathbf{D}_h^E \cdot \nabla e, \tag{2}$$

with $\mathbf{D}_h^E = \mathbf{D}^E + \mathcal{D}^E$ in which $\mathbf{D}^E$ denotes the coefficient of dispersion of E, and $\mathcal{D}^E$ denotes the coefficient of diffusion of E.

The MEL formulation of equation 1 reads

$$\frac{1}{\phi}\frac{\mathrm{D}_{\mathrm{v}}}{\mathrm{D}t}(\phi) + \frac{1}{S}\frac{\mathrm{D}_{\mathrm{v}}}{\mathrm{D}t}(S) + \frac{1}{e}\frac{\mathrm{D}_{\tilde{\mathrm{v}}}}{\mathrm{D}t}(e) = -\nabla \cdot \mathbf{V} + \frac{\mathbf{D}_h^E}{e}:(\nabla\nabla e) - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E, \tag{3}$$

where $\frac{\mathrm{D}_{\mathrm{v}}}{\mathrm{D}t}(..) \equiv \frac{\partial}{\partial t}(..) + \mathbf{V}\cdot\nabla(..)$ denotes the material derivative of (..) associated with a particle carrying (..), moving at a velocity $\mathbf{V}$ along its characteristic curve. Because $\phi S e$ expresses the quantity of E per unit volume of porous medium, the left-hand side of equation 3 describes how this quantity varies along the curve that refers to the movement of the particle.

The velocity that serves as the characteristic velocity for the propagation of e reads

$$\tilde{\mathbf{V}} \equiv \mathbf{V} - \frac{1}{\phi S}\nabla(\phi S \mathbf{D}_h^E). \tag{4}$$

This is referred to as a modified velocity due to spatial variations in ϕ, S, and $\mathbf{D}_h^E$.

We note that equation 4 accounts for the fluid velocity and an apparent velocity term associated with the heterogeneity characteristics of the medium. The first is along a gradient from a higher energy level to a lower one, the latter along a gradient from high hydrodynamic dispersion to a lower one.

Following the Lagrangian concept, e will propagate along a pathline, carried with a particle, defined by

$$\frac{\mathrm{D}_{\tilde{\mathrm{v}}}}{\mathrm{D}t}(\mathbf{r}) = \tilde{\mathbf{V}} \tag{5}$$

where $\mathbf{r}$ denotes a spatial position vector.

We note that in the absence of the velocity (i.e., $\mathbf{V} = 0$), equation 1 will describe the Eulerian form of the flow equation while equation 3 will provide its MEL formulation. The Eulerian, EL, and MEL forms for the flow and the transport equations can be combined to read

$$\frac{1}{\phi}\frac{\mathrm{D}_{\mathrm{v}*}}{\mathrm{D}t}(\phi) + \frac{1}{S}\frac{\mathrm{D}_{\mathrm{v}*}}{\mathrm{D}t}(S) + \frac{1}{e}\frac{\mathrm{D}_{\tilde{\mathrm{v}}*}}{\mathrm{D}t}(e) = -(1 - f - \lambda)\nabla\cdot\mathbf{V} + \varphi\frac{\mathbf{D}_h^E}{e}:(\nabla\nabla e) + \frac{(1-\varphi)}{\phi S e}\nabla\cdot[\phi S(\mathbf{D}_h^E\cdot\nabla e)] - \frac{\lambda}{e}\mathbf{V}\cdot\nabla e - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E, \tag{6}$$

where

$$\tilde{\mathbf{V}}^* \equiv \mathbf{V}^* - \frac{\varphi}{\phi S}\nabla(\phi S \mathbf{D}_h^E); \tag{7}$$

and

$$\mathbf{V}^* \equiv (1 - f)\mathbf{V}. \tag{8}$$

The various Eulerian, EL, and MEL formulations of the flow and transport problems can be obtained by introducing different choices of the f, λ, and φ coefficients in equations 6–8 . These choices are summarized in Table 1.

TABLE 1. CHOICE OF CONTROL COEFFICIENTS

	Eulerian		EL		MEL	
control coef.	Flow	Transport	Flow	Transport	Flow	Transport
f	1	1	/	0	1	0
φ	0	0	/	0	1	1
λ	0	1	/	0	0	0

Why MEL

The numerical schemes of the Eulerian and the EL methods do not specifically address the heterogeneity of the medium, which may be presented in the form of steep gradients of the permeability and/or the dispersion coefficients. For the MEL method this is specifically accounted for as additional information included in the velocity (equation 4) of the particle and thus affects the solution process.

The EL formulation is reported to be effective in overcoming numerical dispersion phenomena when simulating problems that are dominated by advection. In view of equation 4, it is argued that the second term on the right-hand side of equation 4 can also be significant in dictating a situation similar to the advection dominant characteristics. Note that this may occur for governing equations with no reference to $\mathbf{V}$, or even when $\mathbf{V}=0$. Accordingly, as described in Table 1, the EL formulation cannot be implemented to flow problems as in the case of the MEL formulation. We thus suggest that it can be preferable to simulate advection dominated problems by the MEL formulation rather then the EL formulation.

We suggest that in view of equation 1 for a transport equation (similar arguments hold upon referring to the flow equation), when considering the flux $\phi S(\mathbf{D}_h^E \cdot \nabla e)$ for a heterogeneous medium (with steep gradients of $\phi S \mathbf{D}_h^E$), it may be that $|\nabla(\phi S \mathbf{D}_h^E) \cdot \nabla e| \gg |\phi S \mathbf{D}_h^E{:}\nabla\nabla e|$. This will conform equation 1 to become hyperbolic dominant. The validity of this argument is demonstrated in the following.

Mathematical statement

We demonstrate the basic arguments in reference to a one-dimensional case of flow or transport equation. This is done for the sake of simplicity and has no effect on the general conclusions.

The purely hyperbolic, advective, transport problem can be described by

$$\frac{\partial e}{\partial t} + V\frac{\partial e}{\partial x} = f, \tag{9}$$

in which f denotes a source term, V denotes the phase velocity, and e denotes the density of E, an extensive quantity of the fluid phase. On the basis of equation 9 and when accounting for a diffusion-dispersion process, we refer to a parabolic transport equation in the form

$$\frac{\partial e}{\partial t} + V\frac{\partial e}{\partial x} = D\frac{\partial^2 e}{\partial x^2} + f, \tag{10}$$

in which D denotes a generalized diffusion-dispersion coefficient. Note that in terms of the mass flux, $D\,\partial e/\partial x$, equation 10 can be rewritten:

$$\frac{\partial e}{\partial t} + C\frac{\partial e}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial e}{\partial x}\right) + f \tag{11}$$

where

$$C \equiv V + \frac{\partial D}{\partial x}, \tag{12}$$

in which C is regarded as an apparent velocity. This velocity will conform to a similar form as in equations 11 and 12 if the first right-hand side of equation 10 is replaced by $\partial(D\,\partial e/\partial x)/\partial x$, the divergence of the mass flux.

The extent to which an advection-dispersion equation is considered to be advection dominant is commonly related to P_e, the Peclet number. In view of equations 11 and 12, we suggest expanding the definition of P_e to read

$$P_e \equiv \frac{L_c}{D}\left|V + \frac{\partial D}{\partial x}\right|, \tag{13}$$

in which L_c denotes a characteristic length. By virtue of equation 13 we note that a high Peclet number ($P_e \gg 1$), which is associated with an advective dominant equation, can result from steep gradients of D when $V=0$. The latter can be referred to the case of the flow equation for which D is regarded as the permeability coefficient. Hence, equation 13 can be used for both a flow and/or a transport equation. Moreover, the advective-dispersive transport equation can be prescribed with no reference to the fluid velocity. For such a case, the behavior of the transport equation can be investigated only by equation 13. To demonstrate that such a form of a transport equation may exist, we multiply equation 11 by $\Lambda(x) \neq 0$, and assume that

$$\Lambda\frac{\partial}{\partial x}\left(D\frac{\partial e}{\partial x}\right) - \Lambda C\frac{\partial e}{\partial x} = \frac{\partial}{\partial x}\left(D\Lambda\frac{\partial e}{\partial x}\right). \tag{14}$$

The equality between both sides of equation 14 can be ensured if

$$\Lambda C = -D\frac{\partial \Lambda}{\partial x}, \tag{15}$$

which is solved by

$$\Lambda = \Lambda_0 \exp\left[-\int_0^x \frac{C(\eta)}{D(\eta)}d\eta\right]. \tag{16}$$

By virtue of equation 16, we can rewrite equation 11 in the form

$$\Lambda\frac{\partial e}{\partial t} = \frac{\partial}{\partial x}\left(D\Lambda\frac{\partial e}{\partial x}\right) + \Lambda f. \tag{17}$$

We note that equation 11 and 17 are equivalent, although the latter does not contain a velocity term.

Example of a coupled hydrological phenomenon

In the following we describe an example considering the modeling of a coupled hydrological phenomenon, using the MEL method. This will be in terms of the flow, transport, and heat equations representing the saltwater-intrusion problem. The mathematical model is based on the balance equations of momentum and mass for the liquid, mass-balance equation of a solute in the liquid and the solid phases, and energy-balance equation for the porous media.

Eulerian forms. The Eulerian water flow, solute, and heat-transport equations are given as follows. The liquid mass balance equation is

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla\cdot(\phi\rho\mathbf{V}) = \rho_R Q_R - \rho Q_P, \tag{18}$$

where $\phi(p)$ denotes the pressure (p) dependent porosity, $\rho(c, T)$ denotes the liquid density, being a function of solute concentration c (relative to fluid's mass) and fluid temperature T, and ρR denotes the density of a recharged liquid with Q_R as its flux and Q_P as the pumping flux.

Constitutive relations and definitions are

$$\chi_c^\rho \equiv \frac{1}{\rho}\frac{\partial\rho}{\partial c}; \tag{19}$$

$$\chi_T^\rho \equiv \frac{1}{\rho}\frac{\partial\rho}{\partial T}; \tag{20}$$

$$\chi_p^\phi \equiv \frac{1}{1-\phi}\frac{d\phi}{dp}, \tag{21}$$

where χ_c^ρ, χ_T^ρ, and χ_p^ϕ are prescribed at the same reference.

Liquid's linear (Darcy) momentum is

$$\phi\mathbf{V} = -\frac{\mathbf{k}}{\mu}\cdot(\nabla p - \rho\mathbf{g}) = -\mathbf{K}\cdot\left(\nabla H + \frac{\rho-\rho_0}{\rho_0}\nabla Z\right), \tag{22}$$

where $\mathbf{k}$ denotes the intrinsic permeability tensor, $\mathbf{g}$ denotes the vector of gravity acceleration, Z denotes elevation parallel to $\mathbf{g}$, μ denotes the fluid viscosity, $\mathbf{K}(=\mathbf{k}g\rho_0/\mu)$ denotes the hydraulic conductivity, and $H(=p/g\rho_0 + Z)$ denotes an hydraulic head with reference to ρ_0.

Assuming decay with η as the decay coefficient, and adsorption (governed by linear equilibrium isotherm) on the solid matrix, we write the solute mass-balance equation for the porous medium,

$$\frac{\partial}{\partial t}[\phi\rho c + (1-\phi)\rho_s c_s] = -\nabla\cdot[\phi\rho(c\mathbf{V} - \mathbf{D}_h\cdot\nabla c)] - \eta\phi\rho c + c_R\rho_R Q_R - c\rho Q_P, \tag{23}$$

in which $\mathbf{D}_h$ denotes the dispersion tensor, $c_s(=\kappa_d\rho c)$ denotes the concentration on the solid matrix, ρ_s denotes the constant solid density, κ_d denotes the partitioning coefficient (volume of fluid per unit mass of solid), and c_R denotes the concentration of a solute associated with an injected liquid. Another form, replacing equation 23, can be obtained by multiplying equation 18 by c (for $c \neq 0$) and subtracting this product from equation 23. We thus obtain the solute mass-balance equation,

$$\phi\rho\frac{\partial c}{\partial t} + \frac{\partial}{\partial t}[(1-\phi)\rho_s c_s] = \nabla\cdot(\phi\rho\mathbf{D}_h\cdot\nabla c) - \phi\rho\mathbf{V}\cdot\nabla c - \eta\phi\rho c + (c_R - c)\rho_R Q_R. \tag{24}$$

In writing the energy-balance equation for the porous medium, we assume linear thermodynamics. We assume small deformations so that we neglect the energy associated with heat dissipation and with change of volume. Furthermore, the liquid specific heat at constant volume, C_f, and the solid specific heat at constant strain, C_s, are assumed constant. We assume that the liquid and solid temperatures are practically equal, and the solid velocity and its dispersive heat flux are much smaller than that of the liquid. Hence, following Bear and Bachmat (1990), we write the porous medium energy-balance equation,

$$\frac{\partial}{\partial t}\{[\phi\rho C_f + (1-\phi)\rho_s C_s]T\} = -\nabla\cdot\{\phi[(\rho C_f T)\mathbf{V} - \mathbf{D}^{*H}\cdot\nabla(\rho C_f T) - \boldsymbol{\lambda}^*\cdot\nabla T]\} + \rho_R C_f T_R Q_R - \rho C_f T Q_P, \tag{25}$$

where $\mathbf{D}^{*H}$ denotes the liquid thermal dispersion coefficient as suggested by Nikolaevskij (1990) and λ^* (for isotropic medium, $\lambda_{ij}^* \equiv \lambda\delta_{ij}$) denotes the thermal conductivity coefficient of the porous medium.

MEL forms. By differentiating equations 18, 23, and 25 and in view of equations 19 and 22, we can define a matrix form describing the flow, transport, and heat-transfer equations. This reads

$$\mathcal{A}_{ij}\frac{\partial \mathcal{Y}_j}{\partial t} + \mathcal{B}_{ij}\cdot\nabla\mathcal{Y}_j = \mathcal{C}_{ij}{:}\nabla\nabla\mathcal{Y}_j + \mathcal{E}_i, \tag{26}$$

where

$$\mathcal{C} = \begin{bmatrix} (\mathrm{k}/\mu) & 0 & 0 \\ c(\mathrm{k}/\mu) & \phi\mathbf{D}_h & 0 \\ T(\mathrm{k}/\mu) & T\chi_c^\rho\phi\mathbf{D}^{*H} & (1/\rho C_f)\phi\boldsymbol{\lambda}^* + (1+\chi_T^\rho T)\phi\mathbf{D}^{*H} \end{bmatrix}, \tag{27}$$

$$\begin{aligned}
\mathcal{A}_{11} &= (1-\phi)\chi_p^\phi \\
\mathcal{A}_{21} &= c(1-\phi)\chi_p^\phi(1-\rho_s\kappa_d) \\
\mathcal{A}_{31} &= (1-\phi)\chi_p^\phi T\left(1-\frac{\rho_s C_s}{\rho C_f}\right) \\
\mathcal{A}_{12} &= \phi\chi_c^\rho \\
\mathcal{A}_{22} &= (1+c\chi_c^\rho)[\phi + (1-\phi)\rho_s\kappa_d] \\
\mathcal{A}_{32} &= \phi\chi_c^\rho T \\
\mathcal{A}_{13} &= \phi\chi_T^\rho \\
\mathcal{A}_{23} &= c\chi_T^\rho[\phi + (1-\phi)\rho_s\kappa_d] \\
\mathcal{A}_{33} &= \phi(1+\chi_T^\rho T) + (1-\phi)\frac{\rho_s C_s}{\rho C_f}\,.
\end{aligned} \tag{28}$$

$$\mathcal{Y} = \begin{bmatrix} p \\ c \\ T \end{bmatrix};$$

$$\mathcal{E} = \begin{bmatrix} \rho\nabla\cdot(\mathbf{k}/\mu)\cdot\mathbf{g} + (\rho_R/\rho)Q_R - Q_P \\ \rho c\nabla\cdot(\mathbf{k}/\mu)\cdot\mathbf{g} - \eta\phi c + c_R(\rho_R/\rho)Q_R - cQ_P \\ \rho c\nabla\cdot(\mathbf{k}/\mu)\cdot\mathbf{g} + c_R(\rho_R/\rho)T_R Q_R - TQ_P \end{bmatrix}, \tag{29}$$

$$\begin{aligned}
\mathcal{B}_{11} &= -\nabla\cdot(\mathbf{k}/\mu) \\
\mathcal{B}_{21} &= -(\mathbf{k}/\mu)\cdot[(1+c\chi_c^\rho)\nabla c + c\chi_T^\rho\nabla T] - c\nabla\cdot(\mathbf{k}/\mu) \\
\mathcal{B}_{31} &= -(\mathbf{k}/\mu)\cdot[\chi_c^\rho T\nabla c + (1+T\chi_T^\rho)\nabla T] - T\nabla\cdot(\mathbf{k}/\mu) \\
\mathcal{B}_{12} &= -\chi_c^\rho(\mathbf{k}/\mu)\cdot(\nabla p + 2\rho\mathbf{g}) \\
\mathcal{B}_{22} &= -\phi\mathbf{D}_h\cdot(\chi_c^\rho\nabla c + \chi_T^\rho\nabla T) - \nabla\cdot(\phi\mathbf{D}_h) \\
&\qquad - (1+2c\chi_c^\rho)\rho(\mathbf{k}/\mu)\cdot\mathbf{g} \\
\mathcal{B}_{32} &= -(1+2c\chi_c^\rho)\rho(\mathbf{k}/\mu)\cdot\mathbf{g} - \chi_c^\rho T\nabla\cdot(\phi\mathbf{D}^{*H}) \\
\mathcal{B}_{13} &= -\chi_T^\rho(\mathbf{k}/\mu)\cdot(\nabla p + 2\rho\mathbf{g}) \\
\mathcal{B}_{23} &= -2\rho c\chi_T^\rho(\mathbf{k}/\mu)\cdot\mathbf{g} \\
\mathcal{B}_{33} &= -2\rho c\chi_T^\rho(\mathbf{k}/\mu)\cdot\mathbf{g} - \phi\mathbf{D}^{*H}\cdot(\chi_c^\rho\nabla c + 2\chi_T^\rho\nabla T) \\
&\qquad - \nabla\cdot(\phi\mathbf{D}^{*H}) - (1/\rho C_f)\nabla\cdot(\phi\boldsymbol{\lambda}^*)
\end{aligned} \tag{30}$$

On the basis of equations 26–30, we can write the MEL formulation for the flow, transport, and heat-transfer problems:

$$\mathcal{G}_{ij}\frac{\partial \mathcal{Y}_j}{\partial t} + \frac{\mathrm{D}_{\mathcal{B}_{ij}}}{\mathrm{D}t}(\mathcal{Y}_j) = \mathcal{C}_{ij}{:}\nabla\nabla\mathcal{Y}_j + \mathcal{E}_i, \tag{31}$$

in which

$$\mathcal{G}_{ij} \equiv \mathcal{A}_{ij} - 1, \tag{32}$$

and

$$\frac{\mathrm{D}_{\mathcal{B}_{ij}}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + \mathcal{B}_{ij}\cdot\nabla. \tag{33}$$

The solution of equation 31 can be viewed in terms of particles moving along characteristic pathlines, carrying pressure, $(..)_p$, solute's concentration, $(..)_c$, and, $(..)_T$, temperature. Such are the particles which are associated with the flow equation, $(..)^\ell$, with velocities $\mathbf{V}_p^\ell$, $\mathbf{V}_c^\ell$, and $\mathbf{V}_T^\ell$. Particles associated with the solute mass-balance equation, $(..)^s$, have the velocities $\mathbf{V}_p^s$, $\mathbf{V}_c^s$, and $\mathbf{V}_T^s$. Particles associated with the heat-transfer equation, $(..)^H$, have the velocities $\mathbf{V}_p^H$, $\mathbf{V}_c^H$, and $\mathbf{V}_T^H$. In view of equations 32 and 33, we note that these velocities are obtained from the components of $\mathcal{B}$, i.e.,

$$\mathcal{B} \equiv \begin{bmatrix} \mathbf{V}_p^\ell & \mathbf{V}_c^\ell & \mathbf{V}_T^\ell \\ \mathbf{V}_p^s & \mathbf{V}_c^s & \mathbf{V}_T^s \\ \mathbf{V}_p^H & \mathbf{V}_c^H & \mathbf{V}_T^H \end{bmatrix}. \tag{34}$$

Moreover, we note that based on the grid size $\Delta x_\ell (\ell = 1, 2, 3)$, we can define the analogous Pe_{ij} and the analogous Cr_{ij}. In view of equations 27 and 34, these are given by

$$Pe_{ij} \equiv |(\mathcal{B}/\mathcal{C})_{ij}|\Delta x_\ell; \tag{35}$$

where $\forall\, \mathcal{C}_{ij} \neq 0$, and

$$Cr_{ij} \equiv \frac{|\mathcal{B}_{ij}|\Delta t}{\Delta x_\ell}. \tag{36}$$

Numerical analysis

When considering a system of coupled PDEs, we cannot guarantee an Eulerian monotone (i.e., obeys the maximum principle and does not yield spurious oscillations) numerical scheme. In what follows we will prove that the MEL scheme is unconditionally monotonic and is thus well suited for the numerical solution of a coupled set of PDEs formulating hydrological phenomena such as saltwater-intrusion problems.

Let us consider, without loss of generality, a one-dimensional system of PDEs. The general Eulerian formulation can be transformed to read

$$\mathbf{A}\frac{\partial \mathbf{e}}{\partial t} + \mathcal{V}\frac{\partial \mathbf{e}}{\partial x} = \frac{\partial}{\partial x}\left(\mathbf{D}\frac{\partial \mathbf{e}}{\partial x}\right) + \mathbf{F}, \tag{37}$$

where $\mathbf{e}$ (e.g., $\mathbf{e}^T \equiv [p, c, T]$ pressure, concentration, and temperature, respectively) denotes the vector of the unknowns and $\mathbf{A}$ is given by

$$A_{ij} = \begin{cases} 0 & \text{if} \quad i \neq j \\ 0 \text{ or } 1 & \text{if} \quad i = j \end{cases}. \tag{38}$$

The nondivergence form (such forms can also be found, e.g., in Oran and Boris, 1987) of equation 37 is

$$\mathbf{A}\frac{\partial \mathbf{e}}{\partial t} + \mathbf{B}\frac{\partial \mathbf{e}}{\partial x} = \mathbf{D}\frac{\partial^2 \mathbf{e}}{\partial x^2} + \mathbf{F} \tag{39}$$

where

$$\mathbf{B} \equiv \mathcal{V} - \frac{\partial \mathbf{D}}{\partial x}. \tag{40}$$

The MEL formulation of equations 39 and 40 can be written in the form

$$\sum_m \left[G_{\ell m}\frac{\partial e_m}{\partial t} + \frac{d_{\ell m}}{dt}(e_m) \right] = \sum_m D_{\ell m}\frac{\partial^2 e_m}{\partial x^2} + F_\ell; \tag{41}$$

in which $G_{\ell m} \equiv A_{\ell m} - 1$, and

$$\frac{d_{\ell m}}{dt}(e_m) \equiv \frac{\partial e_m}{\partial t} + B_{\ell m}\frac{\partial e_m}{\partial x}, \tag{42}$$

and the pathlines equations reads

$$\frac{d}{dt}(x_{\ell m}) = B_{\ell m}. \tag{43}$$

For the numerical approximation of equations 37 or 41, let us consider uniform, $\Delta t (\equiv t^{k+1} - t^k)$, steps in time ($t^k = k\Delta t$, $k = 0, 1, \ldots,$) and uniform, $\Delta x (\equiv x_{i+1} - x_i)$, spatial increments ($x_i = i\Delta x$, $i = 0, 1, \ldots, N$).

The general implicit difference scheme to approximate equation 37 is

$$\frac{\mathbf{A}\mathbf{e}_i^{k+1} - \mathbf{H}_i^{k+1}\mathbf{e}_i^k}{\Delta t} = \mathbf{R}_i^{k+1}\mathbf{e}_{i-1}^{k+1} - \mathbf{Q}_i^{k+1}\mathbf{e}_i^{k+1} + \mathbf{S}_i^{k+1}\mathbf{e}_{i+1}^{k+1} + \mathbf{F}_i^{k+1}, \tag{44}$$

in which $\mathbf{H}_i^{k+1}$ denotes, possible, nonlinear operators and the approximation of spatial derivatives and source terms was considered on the (x_{i-1}, x_i, x_{i+1}) template. In view of equation 44, if we take $\mathbf{H}_i^{k+1} = \mathbf{A}$, we obtain a possible scheme to approximate equation 37. Hence a Eulerian difference scheme for equation 37 reads

$$\mathbf{A}\frac{\mathbf{e}_i^{k+1} - \mathbf{e}_i^k}{\Delta t} = \mathbf{R}_i^{k+1}\mathbf{e}_{i-1}^{k+1} - \mathbf{Q}_i^{k+1}\mathbf{e}_i^{k+1} + \mathbf{S}_i^{k+1}\mathbf{e}_{i+1}^{k+1} + \mathbf{F}_i^{k+1}. \tag{45}$$

The MEL implicit difference scheme to approximate equation 41 on the (x_{i-1}, x_i, x_{i+1}) template is given by

$$\sum_m \left(G_{\ell mi}^{k+1}\frac{e_{mi}^{k+1} - e_{mi}^k}{\Delta t} + \frac{e_{mi}^{k+1} - {}^k e_{\ell mi}}{\Delta t} \right) = \sum_m D_{\ell mi}^{k+1}\frac{e_{m,i-1}^{k+1} - 2e_{mi}^{k+1} + e_{m,i+1}^{k+1}}{(\Delta x)^2} + F_{\ell i}^{k+1}, \tag{46}$$

in which ${}^k(\ )_i$ denotes a value at the i node associated with the t^k time level, from a backward position defined by equation 43. In view of equation 41, we can rewrite equation 46:

$$\sum_m \left(A_{\ell m}\frac{e_{mi}^{k+1} - e_{mi}^k}{\Delta t} + \frac{e_{mi}^k - {}^k e_{\ell mi}}{\Delta t} \right) = \sum_m (R_{\ell mi}^{k+1}e_{m,i-1}^{k+1} - Q_{\ell mi}^{k+1}e_{mi}^{k+1} + S_{\ell mi}^{k+1}e_{m,i+1}^{k+1}) + F_{\ell i}^{k+1}, \tag{47}$$

in which

$$\mathbf{R}_i^{k+1} = \frac{\mathbf{D}_i^{k+1}}{(\Delta x)^2}; \tag{48}$$

$$\mathbf{Q}_i^{k+1} = 2\frac{\mathbf{D}_i^{k+1}}{(\Delta x)^2}; \tag{49}$$

$$\mathbf{S}_i^{k+1} = \frac{\mathbf{D}_i^{k+1}}{(\Delta x)^2}. \tag{50}$$

Comparing equations 44 and 47, we note that the $\mathbf{H}_i^{k+1}$ operators are obtained by

$$\sum_m H_{\ell mi}^{k+1}e_{mi}^k = \sum_m [A_{\ell mi}e_{mi}^k - (e_{mi}^k - {}^k e_{\ell mi})]. \tag{51}$$

These operators can be nonlinear, depending on the interpolation implemented to obtain ${}^k e_{\ell mi}$ at its backward position.

We now investigate the conditions that will prevent the occurrence of spurious oscillations at the t^{k+1} time level, assuming that these did not exist at the t^k previous time level. Hence, without affecting the general implications, let us set the initial conditions (at each t^k time level and for all i nodal points) to be

$$\mathbf{e}_i^k = 0. \tag{52}$$

To investigate the pure performance of the scheme, we omit the influence of the conditions prescribed at the (x_0, x_N) (say, $x_0 = 0$ and $x_N = 1$) boundaries. Hence, we will set the boundary conditions to be

$$\mathbf{e}(0, t^{k+1}) = 0 \tag{53}$$

and

$$\mathbf{e}(1, t^{k+1}) = 0. \tag{54}$$

Any general initial and boundary conditions can by simple transformation be set to equations 52–54, i.e.,

$$\left.\begin{array}{lllll} \mathbf{e} = \varphi(x) & \text{at} & 0 < x < 1; & t = t^k \\ \mathbf{e} = \gamma_0(t) & \text{at} & x = 0; & t \geq t^k \\ \mathbf{e} = \gamma_1(t) & \text{at} & x = 1; & t \geq t^k \end{array}\right\} \Rightarrow$$

$$\begin{cases} \boldsymbol{\varrho} = \mathbf{e} - \varphi(x) & \text{at} \quad 0 < x < 1; \quad t = t^k \\ \boldsymbol{\varrho} = \mathbf{e} - \gamma_0(t) & \text{at} \quad x = 0; \quad t \geq t^k \\ \boldsymbol{\varrho} = \mathbf{e} - \gamma_1(t) & \text{at} \quad x = 1; \quad t \geq t^k \end{cases}$$

We thus solve equation 37 with $\boldsymbol{\varrho}$ as its vector of unknowns, subject to homogeneous boundary and initial conditions.

Focusing on the characteristic of the numerical schemes for equation 37, let us disregard its source terms, i.e., let $\mathbf{F} = 0$. Hence by substituting equations 52 and 53 and 54 into equation 45 (for the Eulerian numerical scheme) or into equation 47 (for the MEL numerical scheme), we obtain

$$\mathbf{R}_i^{k+1}\mathbf{e}_{i-1}^{k+1} - \mathbf{C}_i^{k+1}\mathbf{e}_i^{k+1} + \mathbf{S}_i^{k+1}\mathbf{e}_{i+1}^{k+1} = 0; \tag{55}$$

$$\mathbf{e}_0^{k+1} = 0; \tag{56}$$

$$\mathbf{e}_N^{k+1} = 0, \tag{57}$$

in which

$$\mathbf{C}_i^{k+1} \equiv \frac{\mathbf{A}}{\Delta \mathbf{t}} + \mathbf{Q}_i^{k+1}. \tag{58}$$

In the following we show that the conditions that guarantee the absent of spurious oscillations for equations 55–57 are given by

$$\|(\mathbf{C}_i^{k+1})^{-1}\mathbf{R}_i^{k+1}\| + \|(\mathbf{C}_i^{k+1})^{-1}\mathbf{S}_i^{k+1}\| \leq 1, \quad i = 0, 1, \ldots, N. \tag{59}$$

Samarsky and Nikolaev (1978) proved that the algorithm to solve for the tridiagonal system of equations 55–57 is given by

$$\mathbf{e}_i^{k+1} = \alpha_{i+1}^{k+1}\mathbf{e}_{i+1}^{k+1} + \beta_{i+1}^{k+1}, \tag{60}$$

in which

$$\alpha_{i+1}^{k+1} = (\mathbf{C}_i^{k+1} - \mathbf{R}_i^{k+1}\alpha_i^{k+1})^{-1}\mathbf{S}_i^{k+1}; \quad i = 1, 2, \ldots, N-1; \quad \alpha_1^{k+1} = 0, \tag{61}$$

$$\beta_{i+1}^{k+1} = (\mathbf{C}_i^{k+1} - \mathbf{R}_i^{k+1}\alpha_i^{k+1})^{-1}\mathbf{R}_i^{k+1}\beta_i^{k+1}; \quad i = 1, 2, \ldots, N-1; \quad \beta_1^{k+1} = 0. \tag{62}$$

Accounting in equation 60 for equations 53 and 54, the homogeneous boundary condition (i.e., $\mathbf{e}_0^{k+1} = 0$), we note in equations 61 and 62 the zero values at node $i = 1$. Furthermore, in view of equation 62 we obtain

$$\beta_i^{k+1} = 0; \quad i = 0, 1, \ldots, N. \tag{63}$$

If equation 59 is fulfilled then in view of equation 61 (Samarsky and Nikolaev, 1978), we have

$$\|\alpha_i^{k+1}\| \leq 1; \quad i = 0, 1, \ldots, N. \tag{64}$$

By virtue of equations 60, 63, and 64 we write

$$\|\mathbf{e}_i^{k+1}\| = \|\alpha_{i+1}^{k+1}\mathbf{e}_{i+1}^{k+1}\| \leq \|\alpha_{i+1}^{k+1}\|\,\|\mathbf{e}_{i+1}^{k+1}\| \leq \|\mathbf{e}_{i+1}^{k+1}\|. \tag{65}$$

Hence, by virtue of equation 65, we prove that the scheme of equations 55–57 is monotonous. Moreover, due to the homogeneous boundary conditions, equation 65 implies that the scheme of equations 55–57 will also yield a unique solution in the form

$$\mathbf{e}_i^{k+1} = 0; \quad i = 0, 1, \ldots, N. \tag{66}$$

Because conditions (59) can be implemented for any arbitrary time step (e.g., $\Delta t \gg 1$), we can, instead of equation 59, refer to conditions in the form

$$\|(\mathbf{Q}_i^{k+1})^{-1}\mathbf{R}_i^{k+1}\| + \|(\mathbf{Q}_i^{k+1})^{-1}\mathbf{S}_i^{k+1}\| \leq 1, \quad i = 0, 1, \ldots, N. \tag{67}$$

In view of equations 48–50 and by virtue of equation 67, we note that (equation 47) the MEL implicit difference equations guarantee a monotonous scheme and are specifically suited to solve coupled PDEs. This, however, is not granted with the Eulerian implicit numerical schemes.

NUMERICAL EXAMPLE

Herein we examine the numerical performance of the MEL scheme in terms of its deviation from an analytical solution and when compared to the results obtained by the Eulerian and the EL schemes.

Consider a fluid with constant density flowing through a horizontal one-dimensional saturated porous matrix. The flow and transport of a single solute, in nondimensional forms of H and c, are, respectively,

$$g\rho\chi_p^{\phi}(1 - \phi)\frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial H}{\partial x}\right), \tag{68}$$

and

$$\frac{\partial}{\partial t}(\phi c) = \frac{\partial}{\partial x}\left[\phi\left(D\frac{\partial c}{\partial x} - Vc\right)\right], \tag{69}$$

where $\phi(p)$ denotes the pressure (p) dependent porosity, ρ denotes the liquid density, K denotes the hydraulic conductivity, g denotes the acceleration of gravity, χ_p^ϕ denotes the matrix compressibility, H denotes the hydraulic head, and c denotes the solute concentration. To solve for H and c, we can consider several possibilities.

Case A: A single Eulerian transport equation

In this case we note that equation 68 is decoupled from 69. The fluid velocity, V, can be solved separately by

$$\phi V = -K\frac{\partial H}{\partial x}, \tag{70}$$

and is then introduced, as a prescribed value, into equation 69. The single transport equation reads

$$\phi\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(\phi D\frac{\partial c}{\partial x}\right) - \phi V\frac{\partial c}{\partial x}. \tag{71}$$

Case B: A single EL transport equation

We follow equation 70; however we rewrite equation 71 in the EL form

$$\phi\frac{\mathrm{D}_V}{\mathrm{D}t}(c) = \frac{\partial}{\partial x}\left(\phi D\frac{\partial c}{\partial x}\right), \tag{72}$$

where

$$\frac{\mathrm{D}_V}{\mathrm{D}t}(..) \equiv \frac{\partial}{\partial t}(..) + V\frac{\partial(..)}{\partial x} \tag{73}$$

denotes the material derivative of (..) associated with a particle carrying (..), moving at a velocity V along its characteristic curve.

Case C: A system of the Eulerian flow and transport equations

We now introduce equation 70 into 69 and thus together with equation 68 we obtain a system of equations in the form

$$g\rho\chi_p^\phi(1-\phi)\frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial H}{\partial x}\right) \tag{74}$$

$$\frac{\partial}{\partial t}(\phi c) = \frac{\partial}{\partial x}\left(\phi D\frac{\partial c}{\partial x} + Kc\frac{\partial H}{\partial x}\right) \tag{75}$$

We note that equations 74–75 are a coupled system of nonlinear PDEs for the solution of the H and c variables. Following equation 17, we can argue that the second parabolic equation 75 accounts for the transport equation without referring specifically to the fluid velocity. Hence, in principle, the set of equations 74 and 75 can be regarded as an EL formulation with a zero velocity assigned to the particles. The major difference in the following MEL formulation is that the additional velocity assigned to the particles will be due to the nondivergence form of the formulation.

Case D: A system of the MEL flow and transport equations

We rewrite the flow equation 68 in the form

$$g\rho\chi_p^\phi(1-\phi)\frac{\partial H}{\partial t} - \frac{\partial K}{\partial x}\cdot\frac{\partial H}{\partial x} = K\frac{\partial^2 H}{\partial x^2}, \tag{76}$$

while the transport equation 75 can be rewritten in the form

$$-\frac{\partial}{\partial x}(Kc)\cdot\frac{\partial H}{\partial x} + \left[\frac{\partial}{\partial t}(\phi c) - \frac{\partial}{\partial x}(\phi D)\cdot\frac{\partial c}{\partial x}\right] = Kc\frac{\partial^2 H}{\partial x^2} + \phi D\frac{\partial^2 c}{\partial x^2}. \tag{77}$$

The MEL form of equations 76 and 77 is

$$[g\rho\chi_p^\phi(1-\phi) - 1]\frac{\partial H}{\partial t} + \frac{\mathrm{D}_{V_H^\ell}}{\mathrm{D}t}(H) = K\frac{\partial^2 H}{\partial x^2} \tag{78}$$

and

$$-\frac{\partial H}{\partial t} + \frac{\partial}{\partial t}(\phi c) + \frac{\mathrm{D}_{V_H^s}}{\mathrm{D}t}(H) + \frac{\mathrm{D}_{V_c^s}}{\mathrm{D}t}(c) = Kc\frac{\partial^2 H}{\partial x^2} + \phi D\frac{\partial^2 c}{\partial x^2}, \tag{79}$$

in which

$$V_H^\ell \equiv -\frac{\partial K}{\partial x}; \tag{80}$$

$$V_H^s \equiv -\frac{\partial}{\partial x}(Kc); \tag{81}$$

$$V_c^s \equiv -\frac{\partial}{\partial x}(\phi D). \tag{82}$$

Let us further assume that $\chi_p^\phi = 0$ (i.e., incompressible matrix and flow with fluid velocity constant in space), K and D are constant values so that equations 71 and 76 become linear PDEs, while equations 74 and 77 are nonlinear.

We note that equations 68 and 69 can be solved analytically. Moreover, case A and case B will require fewer numerical approximations (in terms of interpolations) to obtain the solution for H and c. However, in general, we may need to solve a problem consisting of a nonlinear (coupled) set of PDEs. We will hence compare the numerical solution obtained in cases C and D.

Let us also note that the grid Peclet, Pe, and Courant, Cr, numbers read

$$Pe \equiv \frac{|V|\Delta x}{D}; \tag{83}$$

$$Cr \equiv \frac{|V|\Delta t}{\Delta x}, \tag{84}$$

and are valid for cases A and B. In case D, in view of equation 80, we obtain the analogous Peclet and Courant numbers, in the form

$$Pe_H^{\ell} = 0; \tag{85}$$

$$Pe_H^{s} = \frac{(\partial c/\partial x)\Delta x}{c}; \tag{86}$$

$$Pe_c^{s} = 0, \tag{87}$$

and

$$Cr_H^{\ell} = 0; \tag{88}$$

$$Cr_H^{s} = \frac{K(\partial c/\partial x)\Delta t}{\Delta x}; \tag{89}$$

$$Cr_c^{s} = 0. \tag{90}$$

Comparisons between an analytical solution and the numerical solution for the four cases herein is depicted in Figure 1. We note that the EL and MEL (cases B and D, respectively) yield identical results. However, because the latter is solving a set of nonlinear coupled PDEs, we can thus consider it to be more suitable for the simulation of hydrological problems governed by a set of PDEs. The Eulerian formulation for the coupled PDEs is written in terms of nonlinear parabolic (diffusion) equations. Yet, its numerical scheme produces spurious oscillations and over-/under-shooting errors.

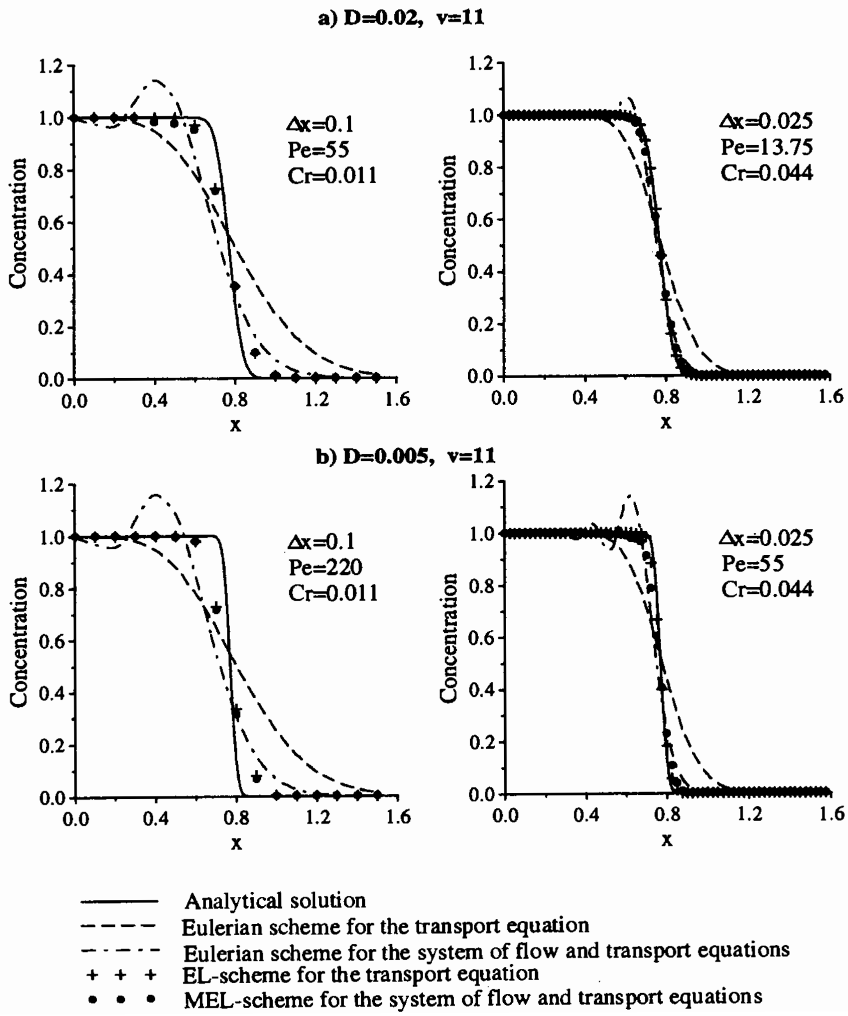

Figure 1. Comparisons ($t = 0.07$) with one-dimensional analytical solution of combined flow and transport equations, for different dispersion coefficients (D), fluid velocities (V), Peclet (Pe), and Courant (CR) numbers.

CONCLUSIONS

A general approach is presented using the MEL formulation to rewrite the governing coupled PDEs of hydrological phenomena. Such models can describe the simultaneous transport of any number of extensive quantities in a porous medium domain that contains multiple multicomponent phases and a deformable solid matrix, under nonisothermal conditions.

In the MEL formulation, each balance equation has the form of a diffusion equation: its left-hand side represents temporal changes, expressed as a linear combination of material derivatives of all intensive variables of the problem. The right-hand side expresses variations in the spatial distributions of the same variables. This takes the form of a linear combination of Laplacians of the same state variables.

Each material derivative involves a velocity of propagation of the particle of the corresponding extensive quantity. These velocities are derived as a modification of the phase (mass weighted) relative velocity, by taking into account heterogeneity in matrix properties (e.g., permeability and porosity), fluid and matrix compressibilities, and spatial changes in surface tension.

The MEL formulation was demonstrated in the case of the coupled nonlinear PDEs exemplified by the hydrological phenomenon of seawater intrusion. In that example we had three extensive quantities: mass of a fluid phase, energy of the porous medium as a whole, mass of a component of the fluid phase in the porous medium, and three state variables, pressure, concentration, and temperature.

A numerical analysis proves that the implicit finite difference approximation of the MEL equations, when applied to a coupled system of PDEs, unconditionally yields a monotonic scheme guaranteeing the absent of spurious oscillations. This is confirmed by a numerical example for the solution of flow and transport of a solute. All parameters were chosen constant and thus an analytical solution was available. Four different solution cases are developed: (a) a single Eulerian transport equation; (b) a single EL transport equation; (c) a coupled system of the Eulerian flow and transport equations; and (d) a coupled system of the MEL flow and transport equations. We note that the grid Peclet, *Pe*, and Courant, *Cr*, numbers are not valid for case c yet following equations 35 and 36, we can define the analog to the grid Peclet and Courant numbers, respectively. The EL and MEL (cases b and d, respectively) yield identical results. However, because the latter is solving a set of nonlinear coupled PDEs, we can consider it to be more suitable for the simulation of hydrological problems governed by coupled PDEs. The Eulerian scheme for case c resulted in spurious oscillations and errors.

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