The "Front Limitation" Algorithm - A New Simulation Technique for Advection - Dispersion Problems

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ABSTRACT

The simulation of multi-phase compositional problems requires the numerical solution of the advection - dispersion equation. Until now the main difficulties were: (1) the mixed types of equation (parabolic and hyperbolic) and (2) the limits in block size and time steps (grid PECLET number, COURANT number). In this paper a new algorithm (named the **FRONT LIMITATION**) is demonstrated which avoids most of the difficulties. The technique makes use of the control volume method with full implicit diffusion-dispersion and source/sink terms and with explicit handling of the advection term. A special front limitation algorithm prevents the known numerical dispersion. The method fulfills the mass balance in each grid element, it has no limits in the grid PECLET number and NEUMANN criterion, has almost no grid orientation effect and has to take account of a low COURANT number and source/sink limits only. The front limitation algorithm can be seen as the basis of a new transport model type with a grid net taking into consideration the geological conditions. The front limitation method will be the basis of a parameter identification technique with sensitivity analysis and the optimal control of source/sink management models.

INTRODUCTION

The simulation of migration processes is one of the most important and interesting tasks of environmental and petroleum sciences. The main reason being, the long characteristic period of the contamination and displacement processes over a period of decades and centuries. Therefore, a prediction can only be done by simulation. It is necessary to mention two other important application fields:

- the identification of transport parameters by means of simulation models;
- the optimal control of sources/sinks and boundary conditions to solve management problems.

Up to now, in the case of many unknown parameters, an excessive amount of computing time renders all methods practically unusable. Therefore, we have developed a finite-difference algorithm for the transport problem which is not limited in the value of the grid Peclet number and overcomes the difficulties connected with the mixed type of parabolic and hyperbolic equations. The Front Limitation algorithm represents a breakthrough in the efficient numerical solution of migration, and, accordingly, in the corresponding parameter identification problem.

THEORY

The simulation of compositional flow is the numerical solution of the transport equation with the dispersion matrix D for the dispersion in an

$$\text{div}(\bar{D} \text{grad } C - \bar{w} C) - k C = S \frac{\partial C}{\partial t} - q \quad (1)$$

isotropic medium, an unsteady state velocity field $w(x,y,z,t)$, a source distribution $q(x,y,z,t)$, the concentration $C(x,y,z,t)$, the first order decay coefficient $k(x,y,z)$ and the storativity $S(x,y,z)$.

The problem of the numerical solution of equation (1) is to bring together the two "opposing" terms of the transport equation (1) - the parabolic dispersion term and the hyperbolic advection term. Until now a satisfactory solution over the full practical range of Peclet number is only possible with Lagrangian methods like the Method Of Characteristics (MOC) and the Random Walk (RW) algorithm (KINZELBACH, 1987; HAEFNER et al., 1992).

Advection - Dispersion Ratio

The Peclet number characterizes the ratio of advective and dispersive flow

$$Pe = \frac{w \cdot L}{D} \quad (2)$$

where L - characteristic scale length. Equation (2) defines the so called grid Peclet number with $L = \Delta x$, Δx equals the grid spacing.

The dispersion is a stochastic process depending on the stochastic structure of the micro pores and - to a much larger extent dependent on the stochastic structure of the geological layers. Therefore, it is not surprising that the FICKIAN dispersion coefficient is flow path dependent after

$$D_l = \delta_l |w| \quad (3)$$

with subscript l for longitudinal and δ -dispersivity.

With a negligible diffusion the Peclet number is

$$P_e = \frac{L}{\delta_l} \quad (4)$$

of the order of magnitude of 100 to 10,000.

DAGAN (1995) and ANDERSON (1995) have shown that the longitudinal dispersivity is of the order of 10 m only in a regional scale and the transversal dispersivity of the order of decimeters. It is to be concluded that it is necessary to take into account a grid Peclet number of the order of 100 at least in a regional scale.

NUMERICAL SIMULATION ART

The matrix methods (FD - Finite Differences or Control Volume, FE - Finite Element) have an advantage due to the fast sparse matrix algorithms. But the main problem - the upper grid Peclet number limit of the order of 2 - forces a very fine grid with a large number of grid points (Kinzelbach & Rausch, 1995). The second limit consists in a maximum Courant number (Equ.5).

$$Co = \frac{w \Delta t}{S \Delta x} \leq (0.5 \dots 1) \quad (5)$$

It should be mentioned that the multi-phase Courant condition is much more restrictive than the linear advective-dispersive Courant condition (Unger et al., 1996). The combination of both limits forces very small time steps due to small block sizes.

If the Peclet number criterion is neglected the existing problems are well known: a large smearing effect (numerical dispersion) by use of the upstream weighting of the advective

term, oscillations by use of the central weighting and a large grid orientation effect.

THE NEW FRONT LIMITATION ALGORITHM

The main problem of all matrix methods is the discretization of the advective term. It requires special attention for the various components of the multi-phase compositional equations. From a physical point of view the advective term describes the movement of a concentration front which is not smooth. Therefore, some authors have suggested flux corrected methods which take into account the mass flow rates and flow directions on the grid cell boundaries by interpolations (Harten 1983, 1988, Michael & Rubin 1991, Rubin & Blunt 1990, Vasiliev 1981, Zalesak 1979, Zazovskij & Musaev 1987).

The idea of our algorithm can be described in the following.

- The advection is dominant which means that there is a miscible displacement process with a steep front. On the other hand, disturbances propagate in all directions in such processes which are described by parabolic equations, but in hyperbolic problems disturbances come from upstream. Therefore, we have to go **upstream** and to **extrapolate** the upstream effect down to the outflow element boundary ($i+1/2$) (s. Fig. 1).
- The result of the displacement process is a concentration distribution. Therefore, we have to extrapolate the concentration C , but not the

mass flow rate (w C).

- The normal upstream weighting is a zero order **extrapolation**. The central weighting is an interpolation method. It is our opinion : **Never to interpolate but to extrapolate**. In Fig. 1 it is shown that the extrapolated curve is influenced by the front only.
- The extrapolation has to be done down to the ($i+1/2$) boundary by a polynomial function.

$$C_{E,i+1/2}(x) = \sum_{i=0}^p a_i x^i \quad (p \leq 2) \quad (6)$$

The polynomial coefficients a_i are determined with the upstream grid points $i, i-1, i-2$ and corresponding state variables, only. We have to prove the monotonicity of the function. The proof can be shown easily in the case of $p \leq 2$.

Then it is necessary to determine the best extrapolation with the following condition :

$$C_{i+1/2} = \text{Min} (\text{MAX}(C_p C_{i+1}), \\ \text{MAX}(\text{MIN}(C_p C_{i+1}), \\ C_{E,i+1/2})) \quad (7)$$

The condition (7) realises limited values for $C_{i+1/2}$ on the grid cell boundary between C_i and C_{i+1} as a maximum or minimum (FRONT LIMITATION). In order to take into account the mass balance in the element i , it is necessary to determine the value $C_{E,i+1/2}$ from the extrapolation in the element ($i-1$). The discretization of the transport equation (1) takes into account the numerical experience with

- * fully implicit or semi-implicit discretization of the dispersion term and the source/sink term,
- * explicit discretization of the advective term.
- * The FRONT LIMITATION weighting is done in each coordinate axis. If the monotonicity of the polynomial (8) is not given, it is convenient to follow the velocity vector upstream (i.e. to follow the path line upstream), or to use a first order polynomial only.

To illustrate the numerical algorithm, table 1 (Appendix) shows the 2D - difference formulation of a diffusion - advection problem. One can see that the difference equation leads to a symmetrical, diagonally-dominant coefficient matrix which can be solved with known solvers.

A similar method is published by Unger et al. (1996). They suggest a Van Leer flux limiter as smoothness sensor which is a spatial weighting function between upstream and downstream points. The differences to our method consists in:

- the application of a smooth weighting function (without physically reasonable approach)
- and the implicit numerical advection-dispersion solution.

This method is also applicable for unstructured grids and multi-phase flow (Unger et al., 1996). Numerical experiments show that for practical problems, upstream weighting of the relative permeability and viscosity terms produces very little numerical dispersion of the saturation shock fronts. In a heterogeneous permeability field macro-dispersion dominates numerical dispersion and a smearing of front does not to be a serious problem. The saturation shock fronts are self-sharpening. On the other hand the compositional flow produces an excessive numerical dispersion of contaminant front (Unger et al., 1996).

VERIFICATION of the FRONT LIMITATION (FL) ALGORITHM

The algorithm has been tested in 1D, 2D (horizontal and vertical cut) and 3D - versions. The verification has been performed using analytical solutions of

- the 1D transport with a first type boundary condition on a semi-infinite path line;
- an areal source in an infinite domain and a volume source in a 3D infinite domain.

In addition, the algorithm has also been verified in comparison with RANDOM WALK simulation runs.

1D Verification

In Fig.2 the comparison of the 1D results with the analytical solution shows an excellent accuracy of the FL algorithm. It has been established that FL does not show an upper grid Peclet number limit. This means there are no limitations in grid block size except from the physical point of view. The grid must be finer than the plume width.

For a small grid Peclet number ($\ll 1$) the Courant number could be larger than 0.5 and even larger than 1. For a grid Peclet number higher than 10 time steps with a maximum Courant number lower than 0.3 should be used. It should be mentioned that the unlimited grid Peclet number removes the known problem of very small time steps necessary because we are now able to use large grid blocks.

2D Verification

With the development of two different 2D tools (horizontal transport with steady state velocity and vertical cut) we were able to test the grid orientation

effect and the influence of a various block size. In Figures 3 an areal source is shown in a principal direction grid. The analytical solution is not available in the inner of the source. The accuracy is sufficient for a large grid Peclet number (1000). A comparison of concentration values along profiles in x- and y-direction through the areal source for a grid Peclet number of 1000 is illustrated in Fig. 4a,b.

Fig.5 shows the areal source in a diagonal grid computed with the analytical solution and FRONT LIMITATION. Comparisons with the "normal" matrix solutions (upstream and central weighting) showed large numerical dispersions and oscillations.

Calculations using upstream and central weighting methods lead to unusable results. The FL algorithm does not show any grid orientation effect. It should be mentioned that a steep concentration front can be simulated between two grid points only. For example, it is possible to simulate a front of 15 m horizontal length with a 10 x 10 m grid. It should be mentioned too, that the numerical solution of a transport problem with a grid Peclet number of 710 was not possible until now. In order to solve this problem (Fig.5) it was necessary to use a grid with more than 2500 x 2500 grid points instead of 25 x 25 grid points (FL).

3D Verification

The 3D-case has been tested with a volume source analytical solution. In addition, we simulated the travelling of a plume in a layered system (Fig. 6a,b). The waste disposal is situated in layer 1, the water wells are situated in layer 1 and 3 and there is a *hydraulic window* in layer 2. The plume has arrived at layer 3. The RANDOM WALK simulation run (25 x 25 m grid) for a five-year period required more than 3 hours CPU time in comparison to 4 minutes (25 x 25 m grid) and 3 seconds (50 x 50 m grid) with FRONT LIMITATION, both on a Pentium PC, i.e. respectively 2% and 0.12% of the original time.

Figure 2. 1D transport with a grid Peclet number of 20 with oscillations in the case of central weighting and numerical dispersion by upstream weighting. Excellent agreement between analytical and numerical FL results. $Pe^* = 20$, $Co = 0.7$, $w = 10^{-5}$ m/s, $t = 4.7 \cdot 10^6$ s..

Figure 3. Areal source in a principal direction grid. Comparison of FRONT LIMITATION with analytical solution. $Pe^* = 1000$, $Co = 0.1$, $w = 10^{-6}$ m/s, $t = 1.5 \cdot 10^8$ s.

Figure 4a. Rectangular profiles along an areal source in a principal direction. Analytical and numerical FL solutions.
- concentration in x-direction,

Figure 4b. Rectangular profiles along an areal source in a principal direction. Analytical and numerical FL solutions
- concentration in y-direction.

Figure 5. Areal source in a diagonal grid. Comparison of FRONT LIMITATION with analytical solution. $Pe = 710$, $Co = 0.1$, $w = 10^{-6}$ m/s, $t = 1.5 \cdot 10^8$ s.

Figure 6b. Migration of pollutants from a waste disposal in a three layer system. Isolines of concentration in the bottom layer. RW method produces two anomalies because of oscillations.

Figure 6a. Migration of pollutants from a waste disposal in a three layer system. Comparison of FL with RANDOM WALK solutions after a five-year period. Isolines of concentration in the top layer.

SUMMARY

The results show strong evidence for the Front Limitation algorithm. It solves the problem with the control volume method, and uses a split operator with an implicit dispersion and an explicit advection term as well as a special front extrapolation technique. FL has obvious advantages concerning CPU-time requirement, accuracy, permissible dimensions of grid net and, as a consequence, application in parameter identification and optimal control. In addition, the total number of the time steps is also reduced using the FL method. As a result, the whole CPU-time requirement is a small percentage of the computational work compared to other methods.

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Symbols

C - concentration
 D - Dispersion tensor
 D - Dispersion coefficient
 k - decay coefficient
 L - scale length
 q - source strength
 s - travel distance
 S - storativity, (porosity * retardation factor)
 t - time
 w - Darcy velocity
 x, y, z coordinates
 δ - dispersivity

Indices

l - longitudinal
 t - transversal

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Appendix**Table 1 2D - difference formulation and polynomial extrapolation**

Difference equation, 2D

$$\begin{aligned} & \frac{1}{\Delta x_i} \left\{ D_{xx} \frac{C_{i+1,j} - C_{i,j}}{\Delta x_i + \frac{1}{2}} + D_{xx} \frac{C_{i,j} - C_{i-1,j}}{\Delta x_i - \frac{1}{2}} + \right. \\ & + D_{xy} \frac{C_{i+\frac{1}{2},j+\frac{1}{2}} - C_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta y_j} - D_{xy} \frac{C_{i-\frac{1}{2},j+\frac{1}{2}} - C_{i-\frac{1}{2},j-\frac{1}{2}}}{\Delta y_j} \left. \right\} + \\ & \frac{1}{\Delta y_j} \left\{ D_{yy} \frac{C_{i,j+1} - C_{i,j}}{\Delta y_j + \frac{1}{2}} + D_{yy} \frac{C_{i,j} - C_{i,j-1}}{\Delta y_j - \frac{1}{2}} + \right. \\ & + D_{yx} \frac{C_{i+\frac{1}{2},j+\frac{1}{2}} - C_{i-\frac{1}{2},j+\frac{1}{2}}}{\Delta x_i} - D_{yx} \frac{C_{i+\frac{1}{2},j-\frac{1}{2}} - C_{i-\frac{1}{2},j-\frac{1}{2}}}{\Delta x_i} \left. \right\} = \\ & = r_i \frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} + k_{ij} C_{i,j}^{n+1} - q_{ij}^{n+1} + \\ & + \frac{(w_1[C])_{i+\frac{1}{2},j}^n - (w_1[C])_{i-\frac{1}{2},j}^n}{\Delta x_i} + \frac{(w_2[C])_{i,j+\frac{1}{2}}^n - (w_2[C])_{i,j-\frac{1}{2}}^n}{\Delta y_j} \end{aligned}$$

FL

with $C_{i+1/2,j}, C_{i-1/2,j}, C_{i,j+1/2}, C_{i,j-1/2}$ in the time step n

calculated by polynomial function (6), by using the condition (7)