A Conservative Galerkin Characteristics Method for Contaminant Transport Problems in Porous Media

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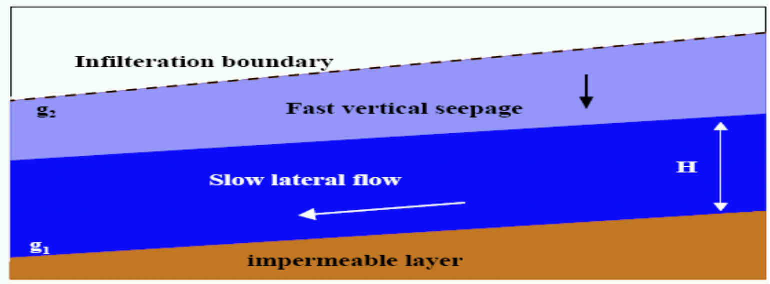
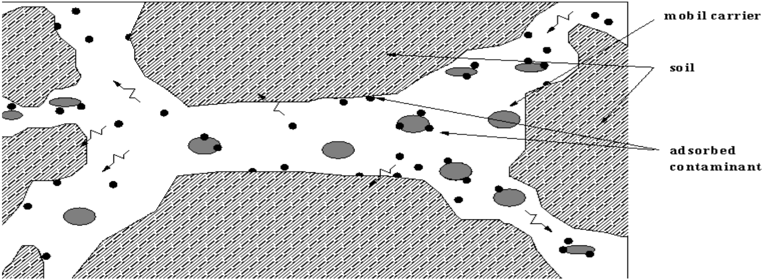
Outline

To get insight into the mechanism of the flow and transport of the fluid in the ground we review some of the the essential physical concepts in porous-media.



Fluid flow processes. H denotes to the height of the ground water tables g_1 , g_2 represent the subsurface and surface topographies, respectively.

Physical considerations



Schematic representation of a porous medium

Kinetic Reaction

The concentration on the solid matrix in general can be due to a number of chemical and biological processes, such as:

1. adsorption (retention/release),
2. ion exchange,
3. dissolution,
4. precipitation,
5. biodegradation.

These can be either: equilibrium, non-equilibrium, or combination of both.

Reactive transport of one contaminant and multi sites

$$\frac{\partial}{\partial t}\{\theta C + \varrho S\} + \nabla \cdot \{qC - D\nabla C\} = G$$

$$S = \sum_{i=1}^{m} \lambda_i S_i, \quad \sum_{i=1}^{m} \lambda_i = 1 \qquad (\lambda_i > 0),$$

$$\partial_t S_i = f(x, C, S_i) = k_i(\psi_i(C) - S_i).$$

The reaction that we will consider is sorption.

C: Concentration of contaminant in the water.

S: Concentration of contaminant on the solid phase.

D and $\rho > 0$: are diffusion tensor and bulk-density.

ψ: Sorption isotherm of porous media with porosity θ.

supplemented by appropriate initial conditions for C and S and boundary conditions for C. We allow for k_i, the rate parameter, to be:

- $k_i < \infty$ for non-equilibrium adsorption whereas ,
- for equilibrium adsorption $k_i = \infty$ and implies that

$$S = \psi(C).$$

Types of isotherm adsorption

The isotherm ψ are sometimes classified according to the behavior near $C = 0$. Well known examples of isotherms are

- the Langmuir isotherm, where

$$\psi(C) = \frac{K_1 C}{1 + K_2 C} \qquad \text{with} K_1, K_2 > 0 \tag{1}$$

- the Freundlich isotherm, where

$$\psi(c) = K_3 C^p \qquad \text{with } K_3, p > 0 \tag{2}$$

Challenging problems

Developing an approximation scheme has to handle the following problems,

- The incorporation of the degenerate nonlinearities of the Freundlich isotherm $\psi'(0+) = \infty$ leading to the solution with sharp front and of finite speed propagation, such that a front given by the boundary of support of C is preserved.
- The convection, associated with the velocity field, dominates the diffusive effects, where the diffusion (in many applications) is of a much smaller magnitude than the convection.

These problems are enough to make most of the numerical schemes unstable, inaccurate, oscillate and have even not physical behavior.

Remedies

- Efficient Regularizaton and relaxation schemes: to control the degeneracy and relax the nonlinearity with few iterations, e.g. Jäger and Kačur (1994, 1996), see also Barrett and Knabner (1993,1998), Mahmood (2008).
- MMOC (Douglas and Russel, 1982, Douglas et al 2000, Pironneau, 1982, Morton, 1988, Bermejo 1995, Arbogas and Huang 2008 and many) is one of the efficient front tracking methods, commonly used for solving different models:
  - is easily applied to multidimensional problems,
  - it is a naturally operating splitting method, other operating splitting methods appear to give a restriction on the time step, or weaken the accuracy.
  - allows large time step.

Moreover, numerical diffusion in MMOC is less than e.g. upwind method.
Unfortunately, in MMOC, mass conservation law is not satisfied and for degenerate nonlinear models the the error in mass balance over time could grow and lead to incorrect approximation solution (unphysical solution).
Fortunately, there are some variants of MMOC which overcome this problem (they are conservative locally or globally), e.g. modified method of characteristics with adjusted advection MMOCAA.
We suggest another variant to MMOCAA which we will call a conservative modified method of characteristics CMMOC.
Eulerian-Lagrangian (localized adjoint ELLAM) and characteristics-mixed finite element method are other variants that conserve mass.

Lagrangian formulation

Our parabolic equation can be rewritten in the form (two sites):

$$\theta\frac{\partial C}{\partial t}+\frac{\partial}{\partial t}\{\varrho_1 S+\varrho_2\psi(C)\}+q\cdot\nabla C-\nabla\cdot(D\nabla C)=0, \tag{3}$$

$$(\theta+\varrho_2\psi')\frac{\partial C}{\partial t}+q\cdot\nabla C-\nabla\cdot(D\nabla C)=-\frac{\partial}{\partial t}\varrho_1 S \tag{4}$$

This can be formulated in Lagragian form as:

$$\frac{db(C)}{dt}-\nabla\cdot(D\nabla C)=-\frac{\partial}{\partial t}\varrho_1 S,\ \frac{d\varphi}{dt}=\frac{q}{b'(C)},\ b(C)=(\theta+\varrho_2\psi'(C)) \tag{5}$$

Where φ represents the characteristics path of a moving particle and $\frac{q}{\theta+\varrho_2\psi'}$ is the velocity of the fluid particle alonge the characteristic.

Memory term

We solve the ODE analytically to get:

$$\partial_t S = k\left[\Psi(C(t)) - \left(S_0\,\mathrm{e}^{-kt} + k\int_0^t \mathrm{e}^{-k(t-s)}\,\Psi(C(s))ds\right)\right] \quad (6)$$

Galerkin-characteristic algorithm can be interpreted as two stages

- The procedure to approximate of convective or transport part and
- the approximation to of diffusion stage.

The semi-descritised regularized model

Let us denote by $C_i \approx C(t_i, x)$ and $b(C_i) = \theta + \varrho_2 \psi'(C_i)$ a variational solution
$t_i = i\tau,\ \tau = \frac{T}{n}, (n \in \mathbb{N}$ and $T > 0$ is a constant). At the instant $t = t_i$ we determine C_i from the sequence of problems of the form:

$$(\lambda_{i,l}(C_{i,l} - C_{i-1} \circ \varphi^i), v) + \tau(D_i \nabla C_{i,l}, \nabla v) + \tau(g_i, v)_{\Gamma_N} = \tau(H_i, v)$$

$$\lambda_{i,l} = \frac{b_n(C_{i,l}) - b_n(C_{i-1})}{C_{i,l} - C_{i-1}}, \qquad \lambda_{i,0} = \theta + \varrho_2 \psi'(C_{i-1}) \qquad (7)$$

for $l = 1, \ldots$. If $|\lambda_{i,l} - \lambda_{i,l-1}|_\infty \le c\tau$ ($c\tau$ is given).

The semi-descritised regularized model

$$b_n(s) = \max\{\tau, \min\{\psi(s), \tau^{-1}\}\} \tag{8}$$

is a regularization of ψ. Approximating of the memory term can be as:

$$(H_i, v) = (-\varrho_1 k \left[\psi(C_{i-1}) - \left(S_0 \,\mathrm{e}^{-kt_i} + k s_i\right)\right], v),$$

$$s_i = \mathrm{e}^{-k\tau} s_{i-1} + \alpha_i \psi(C_i(x)) \quad \text{for } i = 1, \ldots, n,$$

$$\alpha_i = \mathrm{e}^{-k\tau} \int_{t_{i-1}}^{t_i} \mathrm{e}^{-k(t_{i-1}-s)}\, ds.$$

$$\varphi^i = x - \tau \frac{q}{b'(C_{i-1})}.$$

The algorithm for convection stage

The idea has emerged from noticing that the integral involving the product of two piecewise bilinear polynomials in different grids is equivalent to cubic spline interpolation at the knots of the displaced grid along the characteristic curves. The inner product

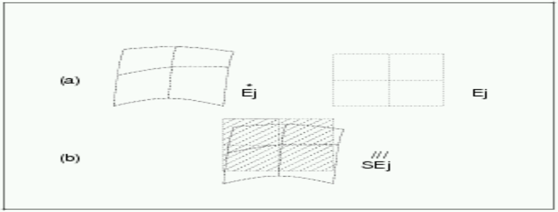
$$(C_{i-1} \circ \varphi^i, \phi_j) = \int_{E_j} C_{i-1} \circ \varphi^i(x) \phi_j(x) dx,$$

where ϕ_j is a basis function, $j = 1, ...P$ and

$$C_{i-1}(x) = \sum_j C_{i-1}^j \phi_j(x).$$

C_{i-1}^j represents the value of the function $C_{i-1}(x)$ at the point x_j. Bermejo (1995) has proposed an accurate and unconditionally stable scheme and it was our interest.

Evaluation of convection part



(a) support E_j of ϕ_j and its image E_j^* (b) support SE_j

CMMOC

The idea behind CMMOC is to adjust the convection, not explicitly as done in, but implicitly so as to minimize the error in the mass balance problem, even for problems of constant coefficients.

$$\int b(C(t_i,x))dx = \int b(C(t_{i-1},\varphi^i))dx \neq \int b(C(t_{i-1},x)dx, \qquad t \geq 0$$

the solution is assumed, for simplicity, to be smooth and to decay rapidly as $|x| \to \infty$.

$$\int b(u(t,x))dx = \int b(u(t_0,x))dx. \tag{9}$$

Then

$$Q^i = \int b(u_i)dx, \quad Q^0 = \int b(u(t_0,x))dx. \tag{10}$$

CMMOC

Such criteria permit us to reduce the error in mass by the following scheme: Define two perturbations of the foot φ^i of the tangent to the characteristics

$$\varphi^i_+ = \varphi^i + \varepsilon h\tau \frac{\bar{q}}{b'(u)},$$

$$\varphi^i_- = \varphi^i - \varepsilon h\tau \frac{\bar{q}}{b'(u)}, \tag{11}$$

where $\varepsilon > 0$ is a fixed constant, chosen to be less than one and h is a spatial discretisation. Then the approximation of the inner products $(b(u_{i-1} \circ \varphi^i_+), v), (b(u_{i-1} \circ \varphi^i_-), v), (b(u_{i-1} \circ \varphi^i), v)$.

CMMOC

As a result we obtain the solutions u_i, u_i^+, u_i^-.
Then, a new u_i can be computed as:

$$u_i = \begin{cases} \max\left(u_i^+, u_i^-\right)\right), & \text{if} \quad Q^i > Q^0, \\ \\ \min\left(u_i^+, u_i^-\right)\right), & \text{if} \quad Q^i \leq Q^0. \end{cases} \tag{12}$$

We repeat the above steps until we get a conservative mass balance error which has to be accepted.

CMMOC

We wish to remark that due to the structure of this scheme, we have got two advantages in comparison with the previous version of MMOCAA.

- On one hand, the mass balance is computed precisely,
- On the other, since the iterative resolution is required for, it turns out that this scheme is not computationally expensive and for constant coefficients model this modification at the end of each time step give us conservation more than the standard MMOC itself.

Discretization and iteration parameters

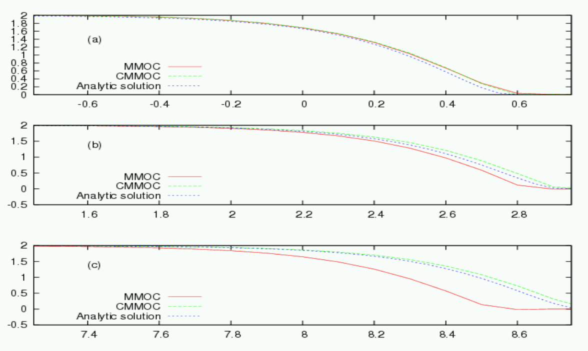
We shall take the following data

- $\theta = 0.5, \rho = 1.5,$
- $\bar{q} = 3, D = 0.05, k = 10,$
- $k_1 = k_2 = k_3 = 1.$

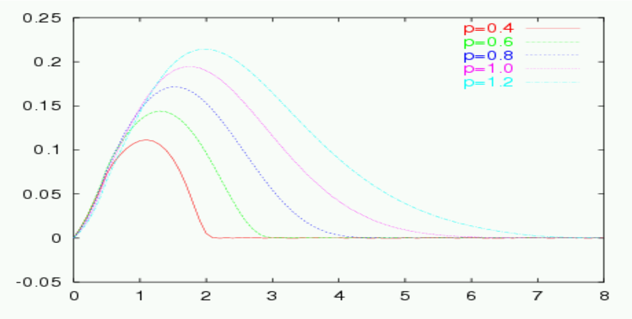
Numerical results

C=CMMOC, S=MMOC

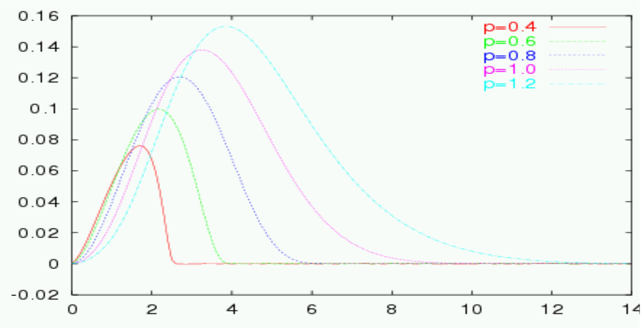
Grid	C	S	C	S	C	S
points	t=1	t=1	t=5	t=5	t=15	t=15
10	1.7e-2	3.3e-2	1.0e-2	3.4e-1	2.3e-2	9.2e-1
20	2.5e-2	1.9e-2	3.8e-2	1.6e-1	1.8e-2	5.4e-1
40	2.2e-2	2.1e-2	1.6e-2	7.9e-2	2.3e-2	2.7e-1
80	2.0e-2	2.0e-2	2.8e-2	2.1e-2	2.8e-2	1.4e-1



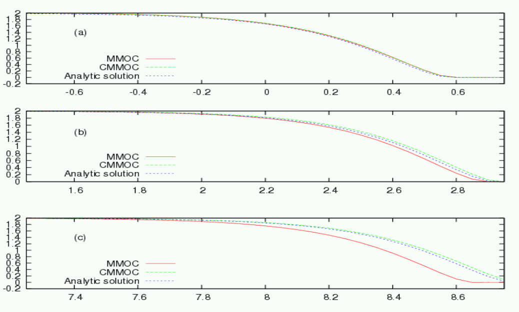
Solution obtained MMOC and CMMOC using 10 grid points at (a) 1 hour (b) 5 hour (c) 15 hours



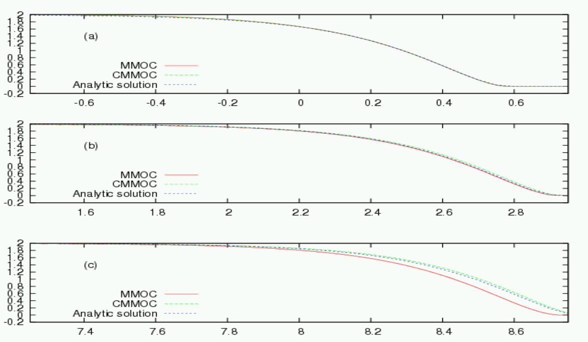
Concentration in nonequilibrium adsorption case at t = 1



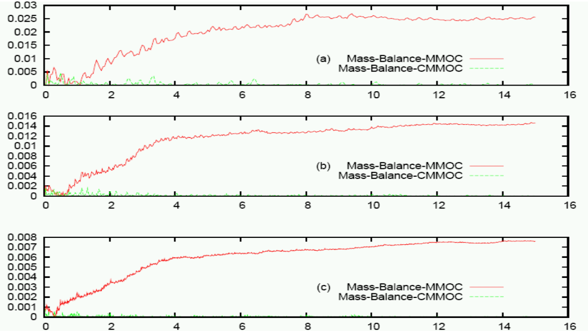
Concentration in nonequilibrium adsorption case at t = 2



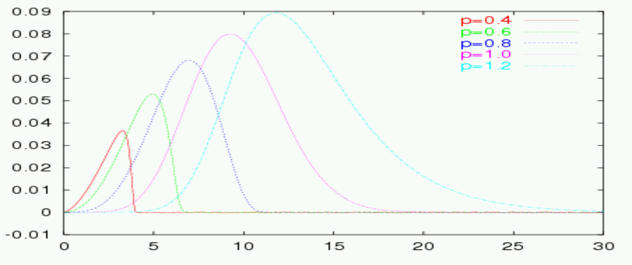
Solution obtained by MMOC and CMMOC using grid points at (a) 1 hour (b) 5 hors (c) 15 hours



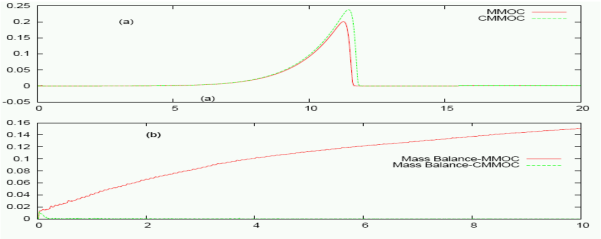
Solution obtained MMOC and CMMOC using 80 grid points at (a) 1 hour (b) 5 hour (c) 15 hours



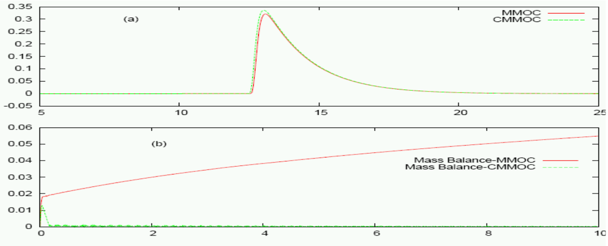
Errors in mass balance obtained by MMOC and CMMOC at 15 hours using (a) 10 grid points (b) 20 grid points (c) 80 grid points



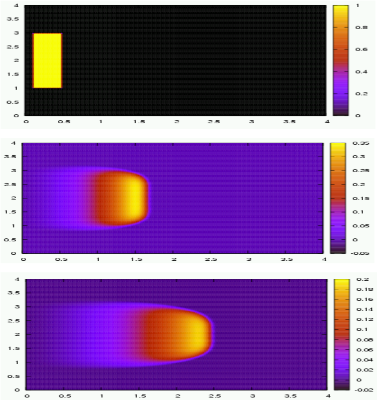
Concentration in nonequilibrium adsorption case at t = 6



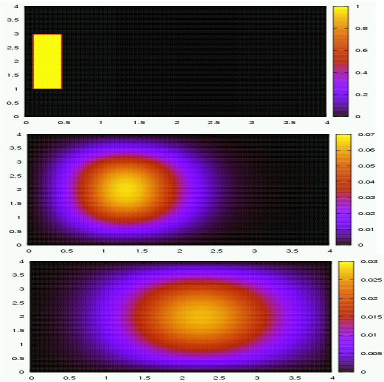
Comparison of (a) the solutions (b) the errors in mass balance



Comparison of (a) the solutions (b) the errors in mass balance



Solution at t = 0,1,2 hours with Freundlich isotherm, p = 0.4



Solution at t=0,1,2 hours with Langmuir isotherms

Theorem

Under suitable assumptions . Then there exists a subsequence of $\{C^n\}$*(again we denote it by* $\{C^n\}$*) such that* $C^n \to u$ *in* $C(I \times \bar{\Omega}) \cap L_2(I, V)$ *if* $N = 1$ *and in* $C(I, L_r(\Omega)) \cap L_2(I, V)$ *(*$r < \frac{2N}{N-2}$ *if* $N > 2, r < \infty$ *if* $N = 2$*) for* $n \to \infty$*. Moreover* C *is a variational solution to our model.*

Theorem

Under suitable assumptions. Then there exits a variational solution $u \in L_\infty(I, V) \cap L_2(I, V)$ *satisfying the variational solution.*

Theorem

Under suitable assumptions. Then

$$\max_{i=0\to N} ||U_i - P_h u||_0^2 + \tau \sum_i^N ||\nabla(U_i - P_h u)||_0^2 \le C(h^2 + t^d). \quad (13)$$

$$d = \begin{cases} 1/3, & N = 3 \\ 1/(2+\varepsilon), & N = 2 \quad (0 < \varepsilon << 1) \\ 1, & N = 1. \end{cases}$$

Conclusion

We have discussed the following

- **Developing an efficient approximation scheme of the considered model and to handel the associated difficulties**
- **Illustrating and validation the behavior and the capability of the schemes by a series of computational experiments.**
- **Deriving error estimates and convergence analysis of the approximated schemes.**

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Thank you