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TRANSPORT THEORY OF HOMOGENEOUS REACTING SOLUTES

ДО ТЕОРІЇ ПЕРЕНЕСЕННЯ ОДНОРІДНИХ РЕАГУЮЧИХ РОЗЧИНІВ

We consider the one-dimensional convection (advection)-dispersion equation of the transport theory of reacting solutes in porous media. A method is given for the best approximation of the numerical solution both in absence of interaction with the solid phase and in presence of discontinuous initial conditions. The class of solutions is determined by the multi resolution analysis of the partial differential operator, using Haar wavelets and splines, and it is compared with the Fourier solution.

Розглядається одновимірне конвекційно-дисперсійне рівняння теорії перенесення реагуючих розчинів у пористому середовищі. Запропонований метод дає найкращу апроксимацію чисельного розв'язку як при відсутності взаємодії з твердими фазами, так і у випадку розривних початкових значень. Клас розв'язків, визначений багатовимірним розподілом змінних та при використанні функцій Хаара та сплайнів, порівнюється з розв'язками, отриманими за методом Фур'є.

1. Introduction. The transport theory of reacting solutes in a porous medium, is a complex phenomenon with different (nonlinear) perturbations (see e.g. [1, 2]). Small changes in the physical parameters have (often) unpredictable consequences on the evolution of the partitioning of the solute between the soil and liquid phase.

The physical-chemical hypotheses of our model are that [1]:

a) the solute transport is taken unidirectional, isothermal and devoid of instabilities;

b) the solute transport takes place in a homogeneous porous medium;

c) the constant, the density and the viscosity of the water in the medium are constant under process;

d) the physical parameters defining the medium are unaffected by the transport (i.e. the size of the pores do not change as well as their distribution in the solid, and so forth);

e) the chemical species defining the solid are immobile (while the chemical species defining the solute are mobile) in the medium.

Let Ω be a one-dimensional domain of $\Re$, x the coordinate of an arbitrary point $x \in \Omega$ and I a finite interval of the time variable t ($I \stackrel{\text{def}}{=} \{T: 0 < t < T,\ T < \infty\}$).

We consider a sufficiently fast and reversible reaction of homogeneous type [1], in particular the solute transport is such that the medium's original solution contains reacting solutes M_1, M_2 and M_1M_2, while the displacing solution contains reacting solutes M_1, M_4 and M_1M_4. The system's transport multiple reaction is represented by the chemical reactions

$$M_1M_2 \rightleftharpoons M_1 + M_2,$$

$$M_1M_4 \rightleftharpoons M_1 + M_4,$$

M_1, M_2, M_4 being the three tenads of the system. The basic equations for the concentrations $c_1, c_2, c_4, c_{12}, c_{14}$ are [1, p. 1235]

$$\Theta \frac{\partial c_1}{\partial t} + \Theta \frac{\partial c_{12}}{\partial t} + \Theta \frac{\partial c_{12}}{\partial t} = Lc_1 + Lc_{12} + Lc_{14},$$

$$\Theta \frac{\partial c_2}{\partial t} + \Theta \frac{\partial c_{12}}{\partial t} = Lc_{12} + Lc_{12},$$

Let $\{V_n\}_{n\in Z}$ be the subset of $L_2(\Re)$ defined as the set of piecewise constant functions $f(x)$ of compact support on D_k^n (n fixed)

$$V_n \stackrel{\text{def}}{=} \left\{f(x)\in L_2(\mathbb{R}):\ f(x)=c_k^n=\text{const}\ \ \forall\, x\in D_k^n,\ \ f(x)=0\ \ \forall\, x\notin D_k^n\right\}.$$

Subsets V_n fulfill the axioms of multi resolution (or multiscale) analysis [3, 4], so that $L_2(\Re)$ is the direct sum of orthogonal subspaces W_n of wavelets

$$\begin{aligned} L_2(\Re) &= \bigoplus_{n\in Z} W_n = V_q \oplus \bigoplus_{j\ge q} W_j, \qquad q\in Z, \\ V_{n+1} &= V_n \oplus W_n, \end{aligned} \tag{8}$$

being $\oplus$ the direct sum of orthogonal spaces. The set of functions $\left\{\Psi_k^n\right\}$, $n\in Z$, represents an orthogonal basis for $L_2(\Re)$ [3].

3.1. Resolution and numerical approximation. Fixing the resolution value $N<\infty$, in (8), the $L_2(\Re)$ space it is approximated by $L_2(\Re)\cong \bigoplus_{n=0}^{N} W_n$, that is,

$$f(x)\cong \pi^{N+1}f(x) \stackrel{\text{def}}{=} \alpha_0^0 + \sum_{n=0}^{N}\sum_{k=0}^{n}\beta_k^n\Psi_k^n(x) \tag{9}$$

being $\pi^n: L_2(\Re)\to V_{n+1}$. The coefficients α_0^0, β_k^n defined as

$$\alpha_k^n \stackrel{\text{def}}{=} \int\limits_{D_k^n} f(x)\Phi_k^n(x)\,dx, \qquad \beta_k^n \stackrel{\text{def}}{=} \int\limits_{D_k^n} f(x)\Psi_k^n(x)\,dx, \tag{10}$$

are easily computed, in the discrete case, by the fast wavelet transform (see e.g. [5]).

Choosing the (dyadic) nodes $x_k \stackrel{\text{def}}{=} k/2^n$, $k=0,\dots,2^n-1$, the dyadic discretization is the operator $\nabla^n: L_2(\Re)\to L_2\left(Z(2^{-n})\right)$ being $L_2\left(Z(2^{-n})\right)\subset L_2(\Re)$ the set of $L_2(\Re)$-functions discretized at x_k. The action of ∇^n on $f(x)$ is such that $\nabla^n f(x)=\mathbf{f}^n$ with $\mathbf{f}^n=\left\{f_0, f_1,\dots, f_{2^n-1}\right\}$ and $\left\{f_k \stackrel{\text{def}}{=} f(x)\big|_{x=x_k},\ 0\le k\le 2^n-1\right\}$. The fast Haar-wavelet transform $\mathcal{H}$ of $\mathbf{f}^n$ is the linear operator [4, 5]

$$\mathcal{H}: L_2\left(Z(2^{-n})\right)\to V_n \,|\, \mathbf{f}^n\mapsto \mathcal{H}\mathbf{f}^n = \left\{\alpha_0^0, \beta_k^n\right\}_{k=0,\dots,n}^{n=0,\dots,2^N-1}, \tag{11}$$

so that, the projection operator $\pi^n: L_2(\Re)\to V_{n+1}$ is factorized as $\pi^n=\mathcal{H}\nabla^n$.

A p-order Cardinal spline, is a $C^{p-2}([0,1))$ differentiable operator

$$\mathcal{S}^p: L_2\left(Z(2^{-N})\right)\to C^{p-2}([0,1)): \mathbf{f}^n\mapsto s(x) \stackrel{\text{def}}{=} \mathcal{S}^p\mathbf{f}^n.$$

A spline Haar derivative is an algorithm [4, 5] such that the differential operator $L: L_2\left(Z(2^{-N})\right)\to L_2\left(Z(2^{-N})\right)$ commutes with $\mathcal{H}$:

$$L\mathcal{H} = \mathcal{H}L\mathcal{S}^p. \tag{12}$$

There follows that, given the set $\mathbf{f}^N$ and computed the spline of sufficiently large order, the spline-derivative of $\mathcal{H}\mathbf{f}^N$ it belongs to the same space of $\mathbf{f}^N$ [4, 5].

The approximate solution of equation (3), up to the resolution N, is the vector $\mathbf{u}^N(\in V_{N+1})$, i.e. assuming the Euler formula for the time-derivative

$$\pi^n \frac{\partial u}{\partial t} = \frac{\mathbf{u}^{N+1} - \mathbf{u}^{N+1}}{\Delta t}$$

we have from (3), $\mathbf{u}^{N+1} = \mathbf{u}^N + \Delta t L(\mathcal{H}\mathbf{u}^N)$ and according to (12)

$$\mathbf{u}^{N+1} = \left(1 + \Delta t \mathcal{H} L \mathcal{S}^p\right)\mathbf{u}^N. \tag{13}$$

With the boundary condition (4), time step $\Delta t = 0.01$, and assuming in $(3)_1$ $Q = D = 1$ and in (4) $a = 1/4$, $b = 1/2$ we obtain after 5 time steps the evolving function of Fig. 2, where, as expected, the concentration tends to a constant value.

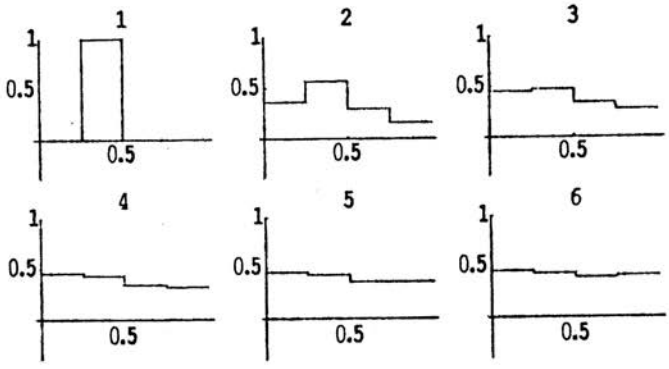

Fig. 2. Haar-wavelet representation of the wave solution

Thus a better modelling of the transport theory of homogeneous reacting solutes is obtained using Haar wavelets combined with splines. We have avoid the Gibbs effect of the Fourier analysis with its lacking of localization of transient functions.

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