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Application of Fem for Solving Thermodispersion Problems in Porous Media

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Introduction

In recent years the theory of thermodiffusion flows in porous media has attracted a considerable atention in connection with environmental problems (Fried, 1975, Goldberg and Gazda, 1984). Because of the comlexity of the problem involving evaluation of initial-boundary value problems for two- and three-dimensional for partial differential equations the most employed turns out to be the numerical approaches to the solution. Untill now the predominant part of works has been devoted to two-dimensional problems (Pinder and Grav, 1973, Petkov, 1984). Moreover, the influence of the temperature and concentration changes on dynamics has not been fully acknowledged in those models and as a rule the transport equation for the diffusion transport in porous media has been solved independently of the solution of heat-conduction equation. The error introduced in such a way is hard to be estimated.
In the present work a numerical method for solving the full conjugated system of thermodiffusion in porous media under the respective boundary and initial conditions is proposed based on a kind of hybrid botween the FEM an FD. A three-dimensional problem is solved for the case of non-homogeneous porous media incorporating the influence of temperature and concentration of the solvent on the hydrodynamic parameters, e. g. Darcy constant, viscosity, etc.
The mathematical model
The transport of heated non-conservative solutes in porous media is governed by the following system of nonlinear partial differential equations (taken in dimensionless form).

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial\left(\frac{c}{\rho}\right)}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_{yy}\frac{\partial\left(\frac{c}{\rho}\right)}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial\left(\frac{c}{\rho}\right)}{\partial z}\right)-\frac{\partial}{\partial x}(u_x c)- \tag{1}$$
$$\frac{\partial}{\partial y}(u_y c)-\lambda R_a c=\frac{\partial c}{\partial t}+\frac{\partial}{\partial t}(u_z c),$$

which is the equation for diffusion in porous media

$$\frac{\partial}{\partial x}\left[M_x\frac{\rho}{\nu}\frac{\partial H}{\partial x}\right]+\frac{\partial}{\partial y}\left[M_y\frac{\rho}{\nu}\frac{\partial H}{\partial y}\right]+\frac{\partial}{\partial z}\left[M_z\frac{\rho}{\nu}\frac{\partial H}{\partial z}\right]=\frac{\partial\rho}{\partial t}, \tag{2}$$

which is derived from continuity equation with substituting in the latter the Darsy low.

$$\sigma \frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right), \tag{3}$$

which is the heat-condition equation.
The equations of state in the considered here case of thermodiffusion are

$$\rho = f_1(c, T); \quad \nu = f_2(c, T), \tag{4}$$

where u_x, u_y, u_z are the components of velocity; c — concentration of the solvent D_{xx}, D_{yy}, D_{zz} — diffusion coefficients; H — hydraulic head; ν — kinematic coefficient of viscosity of the fluid; ρ — density; T — temperature; t — time; α — coefficient of head conductivity. Respectively σ entering (3) stands for the ratio of the thermal capacity of the porous material saturated with fluid to the thermal capacity of the transfer fluid and f_1 and f_2 are functions that are experimentally estimated for the different cases. Also M_x, M_y, M_z are certain dimensionless parameters.

For the diffusivity coefficients we employ the following relations (Petkov, 1984):

$$D_{xx} = \frac{1}{|u|}(\alpha_L u_x^2 + \alpha_T u_y^2 + \alpha_T u_z^2) \tag{5}$$

$$D_{yy} = \frac{1}{|u|}(\alpha_L u_y^2 + \alpha_T u_x^2 + \alpha_T u_z^2) \tag{6}$$

$$D_{zz} = \frac{1}{|u|}(\alpha_L u_z^2 + \alpha_T u_y^2 + \alpha_T u_x^2), \tag{7}$$

where $|u| = \sqrt{u_x^2 + u_y^2 + u_z^2}$, α_L and α_T are geometrical parameters, which depend on the specific properties of the pores of the porous media.
Dimensionless parameter M_x, M_y, M_z are of the form

$$M_x = \frac{k_x t_0 g}{n \nu_0}, \quad M_y = \frac{k_y t_0 g}{n \nu_0}, \quad M_z = \frac{k_z t_0 g}{n \nu_0}, \quad R_a = kg\beta \Delta T H / \nu\alpha, \tag{8}$$

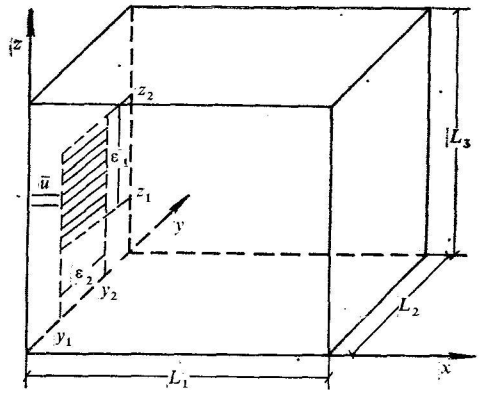


Fig. 1. Region of solution

where n is the porosity of the media, g — gravity acceleration, k_x, k_y, k_z — permiability of coefficients in the directions of x, y, z, respectively.
The heat-conductivity coefficient α is expressed as $\alpha = \frac{k}{\rho c_\rho}$, where c_ρ is the thermal

capacity of the fluid under constant pressure and k is the heat-conductivity coefficient for the system fluid-porous media.
The coefficient σ is

$$\sigma=[c(\rho c_p)_f+(1-c)(\rho c_p)_m]/(\rho c_p)_f. \tag{9}$$

Here the subscript f refers to the fluid, and m — to the porous matrix.
For moderate temperature gradients the most suitable appears to be the well-knwon Boussinesq formula:

$$\rho=\rho_0(1-\beta(T-T_0)), \tag{10}$$

where β is the coefficient of heat dilatation, ρ_0 — density of the pure liquid and T_0 is the temperature at the initial moment of time.
Eqs (1), (2), (3) and (4) comprise a system of conjugated equations in which the velocity field depends on concentration and temperature and vice versa. This system is solved in a region that is parallelopiped of dimensions L_1, L_2 and L_3. For boundary and initial conditions see Fig. 1.

$$c(x, y, z, 0)=0;\quad T(x, y, z, 0)=T_0;\quad H(0, y, z, t)=H_0(z);\quad H(L_1, y, z, t)=H_1(z)$$

$$\left.\begin{aligned} c(0, y, z, t)&=c_0\delta(y-\varepsilon_1)(z-\varepsilon_2)\\ T(0, y, z, t)&=T_1\delta(y-\varepsilon_1)(z-\varepsilon_2)\end{aligned}\right\}\ y_1\leq\varepsilon_1\leq y_2;\ z_1\leq\varepsilon_2\leq z_2.$$

$$\left.\frac{\partial c}{\partial y}\right|_{y=0;\,L_2}=\left.\frac{\partial c}{\partial z}\right|_{z=0:\,L_3}=0;\quad \left.\frac{\partial H}{\partial y}\right|_{y=0;\,L_2}=\left.\frac{\partial H}{\partial z}\right|_{z=0;\,L_3}=0;\quad \left.\frac{\partial T}{\partial y}\right|_{y=0;\,L_2}=\left.\frac{\partial T}{\partial z}\right|_{z=0;\,L_3}=0.$$

Numerical method

For the numerical solution of the above stated problem we employ a combination of the FD and FEM. For each given z stage the respective planar problem is solved by means of method of finite elements and after that by means of finite differences in t direction is solved the full three-dimensional problem.
We use Galerkyn-type FEM and the unknowns H, C and T are sought in the form

$$H=\sum_{i=1}^{NH}H_i\varphi_i(x, y),\quad c=\sum_{i=1}^{NH}c_i\varphi_i(x, y);\quad T=\sum_{i=1}^{NH}T_i\varphi_i(x, y), \tag{11}$$

where NN is the number of grid points and φ_i are the basic functions (Fig. 2, Fig. 3). In the present paper triangular FE with linear approximation are employed.

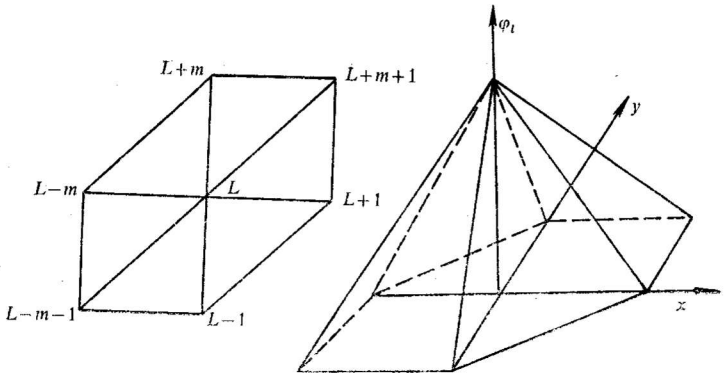


Fig. 2. Triangulation of the region
Fig. 3. Shape of the functions

As usual, making use of Galerkin procedure and Green theorem Eqs (1), (2), (3) are transformed to the following:

$$\int_0^1\int_0^1\Big(D_{xx}\frac{\partial c_k}{\partial x}\frac{\partial\varphi_l}{\partial x}+D_{yy}\frac{\partial c_k}{\partial y}\frac{\partial\varphi_l}{\partial y}-D_{xx}\frac{c_k}{\rho}\frac{\partial\rho}{\partial x}\frac{\partial\varphi_k}{\partial x}-D_{yy}\frac{c_k}{\rho}\frac{\partial\rho}{\partial y}\frac{\partial\varphi_k}{\partial y}+M_x\frac{c_k}{\nu}\frac{\partial H_k}{\partial x}$$

$$\frac{\partial\varphi_l}{\partial x}+M_y\frac{c_k}{\nu}\frac{\partial H_k}{\partial y}\frac{\partial\varphi_l}{\partial y}+\frac{\partial c_k}{\partial t}\varphi_l\Big)\,dxdy+\int_\Gamma\Big[\Big(D_{xx}\frac{c_k}{\rho}\frac{\partial\rho}{\partial x}n_x+D_{yy}\frac{c_k}{\rho} \tag{12}$$

$$\frac{\partial\rho}{\partial y}n_y-M_x\frac{c_k}{\nu}\frac{\partial H_k}{\partial x}n_x-M_y\frac{c_k}{\nu}\frac{\partial H_k}{\partial y}n_y\Big)\varphi_l\Big]d\Gamma=0$$

$$\int_0^1\int_0^1\Big(M_x\frac{\rho}{\nu}\frac{\partial H_k}{\partial x}\frac{\partial\varphi_l}{\partial x}+M_y\frac{\rho}{\nu}\frac{\partial H_k}{\partial y}\frac{\partial\varphi_l}{\partial y}+\frac{\partial\rho}{\partial t}\varphi_l\Big)\,dx\,dy=0, \tag{13}$$

where Γ is the boundary of the region under consideration and n_x, n_y, n_z are the components of the normal to the vector. Compounding the approximations of the different equations we obtain the following system of linear algebraic equations:

$$[N]\{C\}+[M]\left\{\frac{\partial c}{\partial t}\right\}+\{F\}=0 \tag{14}$$

$$[P]\{H\}+[R]\left\{\frac{\partial\rho}{\partial t}\right\}+\{V\}=0 \tag{15}$$

$$[S]\{T\}+[Q]\left\{\frac{\partial T}{\partial t}\right\}+\{W\}=0, \tag{16}$$

where N, M, P, R, S, Q are $(NN-QQ)\times(NN-QQ)$ matrices; QQ-is the number of the grid points for boundary conditions and (c), (H), (T) $\left\{\frac{\partial c}{\partial t}\right\}$; $\left\{\frac{\partial T}{\partial t}\right\}$; $\left\{\frac{\partial\rho}{\partial t}\right\}$ are vectors of the unknown set functions by means of Krank-Nicolson scheme. After the solution at each t-stage if found then we solve the following finite difference scheme:

$$\frac{c^{n+1/2}_{k,l,m}-c^{n+1/3}_{k,l,m}}{0{,}5\Delta t}=\frac{1}{(\Delta z)^2}\Bigg[\Bigg(\frac{\rho^{n+1/3}_{k,l,m+1}+\rho^{n+1/3}_{k,l,m}}{0{,}5}\Bigg)\Big(D^{n+1/3}_{zz\,k,l,m+1}+D^{n+1/3}_{zz\,k,l,m}\Big)\times$$

$$\Bigg(\frac{c^{n+1/2}_{k,l,m+1}}{\rho^{n+1/3}_{k,l,m}}-\frac{c^{n+1/2}_{k,l,m}}{n+1/3}\Bigg)-\Bigg(\frac{\rho^{n+1/3}_{k,l,m}+\rho^{n+1/3}_{k,l,m-1}}{2}\Bigg)\Bigg(\frac{D^{n+1/3}_{zz\,k,l,n}+D^{n+1/3}_{zz\,k,l,m-1}}{2}\Bigg)\times \tag{17}$$

$$\Bigg(\frac{c^{n+1/2}_{k,l,m}}{\rho^{n+1/3}_{k,l,m}}+\frac{c^{n+1/2}_{k,l,m}}{\rho^{n+1/3}_{k,l,m-1}}\Bigg)\Bigg]-\Bigg(\frac{u^{n+1/3}_{z_{k,l,m+1}}c^{n+1/2}_{k,l,m}-u^{n+1/3}_{z_{k,l,m}}c^{n+1/2}_{k,l,m}}{\Delta z}\Bigg)-\lambda Rdc^{n+1/2}_{k,l,m}$$

For Eqs (2) and (3) are constructed similar implicit schemes that appear to be unconditionally stable. In order to obtain the full approximation the explicit corrector scheme is used:

$$\frac{c^{n+1}_{k,l,m}-c^{n}_{k,lm}}{\Delta t}=Ac^{n+1/2}_{k,l,m}-\lambda Rdc^{n+1/2}_{k,l,m}, \tag{18}$$

where A is the net difference operator.

The implementation of the above-described numerical method includes varilable space increments that account, in sense, for the presense of the abrupt changes in concen-

tration profile (the front of concentration). For instance, at a given stage the grid points in the respective (x, y) plane are chosen to be more dense in the region $0 \leq x \leq L_{xt}$, where $L_{xt} = u_x(t + nd)$, $n = 0, 1, 2$. Respectively, their number is much smaller for $L_{xt} < x \leq 1$ since the front of concentration has not reached yet this region and quantities of concentration and temperature remain constant. In our case the velocity

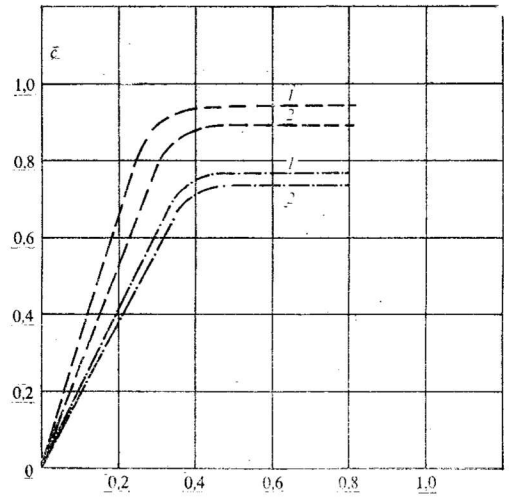


Fig. 4. Comparison between numerical solutions and analytical solutions $M_x = 0{,}9616$; $M_y = 0{,}02054$; $M_z = 0{,}00724$, $H_0(z) = 1 + z$; $H_1(z) = 0{,}13 + z$; $D_{xx} = 0{,}00639$; $D_{yy} = 0{,}000046$; $D_{zz} = 0{,}000058$; $u_x = 0{,}192$; $u_y = u_z = 0$; $R_d = 1$; $\lambda = 0$; $R_a = 0$

1/Author's solution

2/Analytical solution

(—·—·—) Linear source $\frac{\varepsilon_1}{L_3} = 0{,}25$; $\varepsilon_2 = 0$;

(- - -) Plane source $\frac{\varepsilon_1}{L_3} = 0{,}25$; $\frac{\varepsilon}{L_2} = 0{,}35$.

component u_x is predominant, i. e. $u_x > u_y$ and $u_x > u_z$ and for this reason u_x is selected to govern the mesh size. Such a procedure allows us to significantly decrease the requirement for computer memory and computational time without compromiting the accuracy.

The algorithm is taken into four iterational steps and thinking ρ^n, c^n, H^n, T^n, ν^n as as known at given time stage t^n we calculate their values at stage t^{n+1} as follows:

(*i*) $H^{n+1}(x, y, z^{n+1})$ is evaluated from (15), where is taken $\frac{\partial \rho^n}{\partial t} = (\rho^n - \rho^{n+1})/\Delta t$.

(ii) The velocity is computed from Darcy law:

$$u^{n+1}(x, y, z, t^{n+1}) = k \nabla H^{n+1}.$$

(iii) With u^{n+1} known. Eqs (14) and (16) are solved for C and T, respectively. In (14), (16) forward differences for the time derivatives are used, i. e.

$$\frac{\partial c^{n+1}}{\partial t} = (c^{n+1} - c^n)/\Delta t.$$

(iv) From the equations of state (4) ρ^{n+1}, ν^{n+1} are defined on the base of computed c^{n+1} and T^{n+1}.

These iterations are repeated for each new time step until convergence is attained. By means of the method and numerical scheme proposed of the porous media and the fluid are under consideration. In Fig. 4 the comparison with the analytical solution for semi-infinite region is shown, when the sources are limited at the line or rectan-

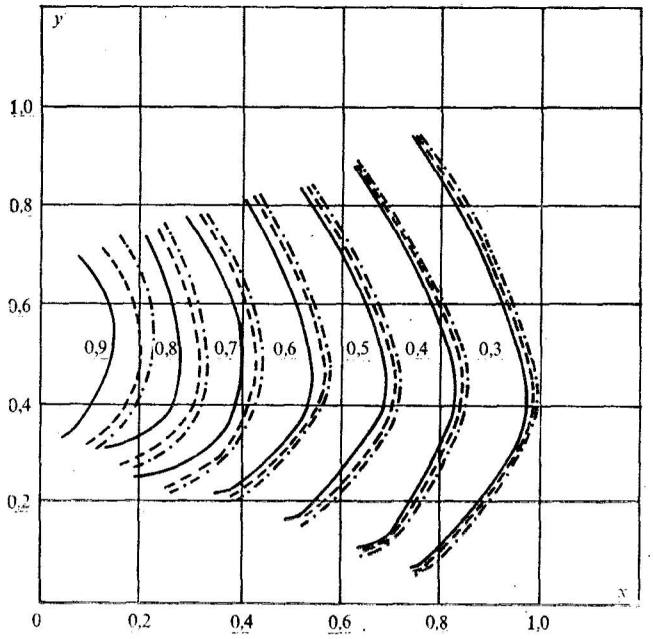


Fig. 5. Lines of equal concentration for variable density and viscosity

$M_x=0{,}9616$; $M_y=0{,}02054$; $M_z=0{,}00724$;
$H_0(z)=1+z$; $H(z)=0{,}13+z$; $\nu_0=0{,}0101$ cm^2/s;
$\rho=1$g/cm^3, $n=0{,}4$; $\frac{\varepsilon_1}{L_3}=0{,}25$; $\frac{\varepsilon_2}{L_2}=0{,}35$;
$z=0{,}5$; $\alpha_L=4$; $\alpha_T=2$.
(———) $\rho=\rho_0$; $\nu=\nu_0$, $R_a=0$;
(- - -) $\rho=\rho_0(1+\beta(T-T_0))$; $\nu=-0{,}5c+1$; $R_a=0$;
(- · - · -) $\rho=\rho_0(1-\beta(T-T_0))$; $\nu=-0.3c-0{,}4T+1$,
$R_a=100$.

gular in the cross-section ($z=1/3$), (Sagar, 1982, Prakash, 1984). It is seen that the numerical solution is obtained on a finite region. The latter ensures us that the numerical method proposed performs well for the three-dimensional problems considered. Here is to be mentioned that in the last comparison the density and viscosity are kept constant during the computations in order to satisfy the conditions under which the analytical solution is obtained.

In Fig. 5 results concerning numerical experiments with variable density and viscosity obeying Eq. (4) are presented. It is well seen that if the viscosity of the liquid increases with concentration and temperature, then the speed propagation of the solute is lowered and vice versa: decreasing the viscosity with it and results in decreasing the speed of propagation of the solute. The specific solvent for results in Fig. 5 is 20% NaCl. The various numerical experiments show that if the viscosity of the mixture in the

initial moment of time does not differ more than 20% from that of pure liquid then the influence on the dynamics and transport can be neglected, i. e. one can solve then the problem with constant density and viscosity. Concerning the density the interval in which the influence can be discarded is about 40%, if the effect of forming layers with different densities is not taken into account.

Conclusions

In the present paper a mathematical model for the thermodiffusion in porous media is proposed for the general case of variable density and viscosity of the mixture. A hybrid FEM/FD numerical method employing variable space increments is compounded for solving the respective equations. Results are obtained for various initial concentrations of the solvents and different equations of state. On the base of the results obtained the regions of variations of density and viscosity are defined in which their influence can be neglected and the simplified model with constant parameters can be used.

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