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CONTINUUM MECHANICS

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On the Numerical Solution of a Class of Diffusion and Sorption Problems

1. Introduction

The simultaneous diffusion and sorption of a substance in porous media is of importance in many transfer operations, taking place in soil, ion-exchange resins, packed bed catalytic reactors, some building and biological materials. The various equations describing the internal diffusion and sorption of one component into a porous body [1], [2], [3] can be presented in the following general form:

$$\frac{\partial c_f}{\partial t} = div(D\ \mathbf{grad} c_f) - \frac{\partial c_a}{\partial t} \quad \text{in } \mathcal{V} \text{ for } t > 0 \tag{1}$$

$$\frac{\partial c_a}{\partial t} = \gamma(\varphi(c_f) - c_a) \tag{2.a}$$

or

$$\frac{\partial c_a}{\partial t} = \varphi_{ir}(c_f) \quad \text{in } \mathcal{V} \text{ for } t > 0 \tag{2.b}$$

where:

c_f is concentration of the free to diffuse substance;

c_a is concentration of the adsorbed part of the substance;

γ is the kinetic parameter corresponding to the desorption rate in case of linear sorption isotherm;

φ is sorption equilibrium isotherm;

φ_{ir} is the irreversible reaction rate function;

D is free species diffusivity which can be:

1. D = const.; 2. $D = D(c_f)$ [3]; 3. $D = D(t)$ and/or $D = D(x,y,z)$.

$\mathcal{V}$ is domain of the space variables, occupied by the body.

The following types of boundary and initial conditions corresponding to different physical assumptions can be imposed:

$$c_f = \Psi_1 \qquad \text{on } S_1 \subset \partial\mathcal{V}, \tag{3.1}$$

$$\mathbf{J}.\mathbf{n} = \Psi_2 \qquad \text{on } S_2 \subset \partial\mathcal{V}, \tag{3.2}$$

$$\mathbf{J}.\mathbf{n} = h(c_f - \Psi_3) \qquad \text{on } S_3 \subset \partial\mathcal{V}, \tag{3.3}$$

$$\mathbf{J}.\mathbf{n} = l\frac{\partial c_f}{\partial t} \qquad \text{on } S_4 \subset \partial\mathcal{V}, \tag{3.4}$$

and

$$c_f = c_f^o(x, y, z), \quad c_a = c_a^o(x, y, z), \quad t = 0 , \tag{4}$$

where: $\mathbf{J} = -D\ \mathbf{grad}\ c$; $S_1 \cup S_2 \cup S_3 \cup S_4 = \partial\mathcal{V}$;

$\mathbf{n}$ is the unite vector normal to S_i, i=1,2,3,4;

$\partial\mathcal{V}$ is the boundary of the domain $\mathcal{V}$;

h, l are parameters, connected with the physical conditions;

Ψ_1, Ψ_2, Ψ_3, c_f^o , c_a^o are known functions.

Eq. (1) and (2.a,b) with the variety of boundary and initial conditions determine one class of boundary value problems.

Solutions of such problems have been investigated in many papers [3] - [12]. They are usually considered in very special symplified situations (as one-dimensional diffusion, linear reaction, sorption equilibrium, steady-state diffusion) to be solved by the conventional analytical methods as separation of variables and finite integral transformations. The general analytical solutions for three-dimensional diffusion and first order reversible reaction into a porous body are obtained in [6]. The one-dimensional nonlinear problems are solved numerically by the finite difference method or the collocation method and analitically under assimptotic conditions [3], [8], [11]. Lately some authors prefere to use numerical or semi-analytical methods even in case of linear equations [5], [9], [10] as the analyticaly expressed concentrations are calculated very tedious.

The aim of the present paper is to propose a different approach to the numerical solution of the above class of problems based on the finite element method (FEM) in a combination with an appropriate time differencing scheme. This approach allows the development of more general numerical algorithms for problems in a domain of arbitrary geometry and under different D, φ, φ_{ir}, Ψ_i.

2. Numerical methods

The numerical solution of the problems (1-4) is sought in the FE form [13]:

$$\bar{c}_f(x, y, z, t) = \sum_{i=1}^{M} N_i(x, y, z) c_f^i(t) , \tag{5}$$

$$\bar{c}_a(x, y, z, t) = \sum_{i=1}^{M} N_i(x, y, z) c_a^i(t) , \tag{6}$$

where: N_i, $i = 1, ..., M$ are the nodal shape functions;

M is the nodes number;

c_f^i, c_a^i are the corresponding values at i-th node;

x, y, z are Cartesian coordinates of a point in $\mathcal{V}$;

t is the time variable.

The FE approximation of the diffusion equation is done in accordance with the Galerkin principle [13]:

$$\int_{\mathcal{V}} N_p \left[\frac{\partial \bar{c}_f}{\partial t} + \frac{\partial \bar{c}_a}{\partial t} - div\mathbf{grad}(\bar{D}\, \bar{c}_f) \right] dv = 0, \quad p = 1,...,M , \tag{7}$$

where $\bar{D} = \sum_{i=1}^{M} N_i D^i$, $D^i = D(x_i, y_i, z_i)$ or $D^i = D(c_f^i)$.

A set of ordinary differential equations is derived from (2)-(7) in the matrix form:

$$\mathbf{CM}^* \frac{d\mathbf{C}_f}{dt} + \mathbf{ST}^* \mathbf{C}_f + \mathbf{CM} \frac{d\mathbf{C}_a}{dt} + \mathbf{F} = \mathbf{O} , \tag{8}$$

$$\frac{d\mathbf{C}_a}{dt} = \gamma(\varphi(\mathbf{C}_f) - \mathbf{C}_a)) \tag{9.a}$$

or

$$\frac{d\mathbf{C}_a}{dt} = \varphi_{ir}(\mathbf{C}_f) \tag{9.b}$$

under the initial conditions

$$\mathbf{C}_f = \mathbf{C}_f^o , \quad \mathbf{C}_a = \mathbf{C}_a^o , \quad t = 0 , \tag{10}$$

where $\mathbf{CM}_{ij}^* = \mathbf{CM}_{ij} + l \int_{S_4} N_i N_j \, ds$, $\mathbf{CM}_{ij} = \int_{\mathcal{V}} N_i N_j \, dv$,

$$\mathbf{ST}^{*}_{ij} = \mathbf{ST}_{ij} + h\int_{S_4} N_i N_j ds\ ,\quad \mathbf{ST}_{ij} = \int_{\mathcal{V}} \bar{D}\ \mathbf{grad}N_i\ \mathbf{grad}N_j dv$$

$$\mathbf{F}_i = \int_{S_2} \Psi_2 N_i ds \ - \ h\int_{S_3} \Psi_3 N_i ds\ ,$$

and $\mathbf{C}_{fi} = \Psi_1(x_i, y_i, z_i)$ for every i being a number of a node on S_1.

The time variable interval $(t_o,\ t_f)$ is descretized by the time differencing mesh $(t_o,\ t_1,\ ...,\ t_N = t_f)$, where $t_n = t_{n-1} + \Delta_n$, n = 1, ..., N and t_f is the final moment under consideration. Eq. (8), (9 a,b) are integrated in the interval $[t_n,\ t_{n+1}]$ by using the trapezoid and the triangle quadrature formulae [14] (assuming the first and second time derivatives of D, $\mathbf{C}_f$, $\mathbf{C}_a$, Ψ_i to be continuous for $t > 0$):

(11) $$\mathbf{CM}^{*}(\mathbf{C}_f^{n+1} - \mathbf{C}_f^{n}) + \Delta_{n+1}/2(\mathbf{ST}^{*}_{n+1}\mathbf{C}_f^{n+1} + \mathbf{ST}^{*}_{n}\mathbf{C}_f^{n}) +$$

$$+ \mathbf{CM}\ (\mathbf{C}_a^{n+1} - \mathbf{C}_a^{n}) \ + \ \Delta_{n+1}\mathbf{F}^{n+0.5} = \mathbf{O}_1(\Delta^3_{n+1})\ ,$$

(12.a) $$\mathbf{C}_a^{n+1} - \mathbf{C}_a^{n} = \gamma\Delta_{n+1}(\varphi(\mathbf{C}_a^{n+0.5}) - \mathbf{C}_a^{n+1}/2 - \mathbf{C}_a^{n}/2\ ) + \mathbf{O}_2(\Delta^3_{n+1}),$$

(12.b) $$\mathbf{C}_a^{n+1} - \mathbf{C}_a^{n} = \Delta_{n+1}(\varphi_{ir}(\mathbf{C}_a^{n+0.5})) + \mathbf{O}_3(\Delta^3_{n+1}),$$

where: $\mathbf{C}_f^k$, $\mathbf{C}_a^k$, $\mathbf{F}^k$ and $\mathbf{ST}^{*}_k$ denote the corresponding vectors at the moment t_k $(t_{k+0.5} = t_k + \Delta_{n+1}/2)$; $\mathbf{O}_i$, i = 1, 2, 3 are linear and bounded vector functions.

The resulted from (11)-(12.a,b) scheme of the Crank-Nicolson type leads to nonlinear algebraic equations in case of a nonlinear sorption (i.e. φ or φ_{ir} is a nonlinear function) and of a nonlinear diffusion (i.e. $D = D(t)$ or $D = D(c_f)$). Eq. (11) and (12.a,b) can be reduced to linear one approximating $\mathbf{ST}^{*}_{n+1}$, $\varphi(\mathbf{C}_f^{n+1})$, $\varphi_{ir}(\mathbf{C}_f^{n+1})$ by $\mathbf{ST}^{*}_{n}$, $\varphi(\mathbf{C}_f^{n})$, $\varphi_{ir}(\mathbf{C}_f^{n})$ with an error of the type $\mathbf{O}(\Delta_{n+1})$. The following one-step difference equation is obtained (with a second order accuracy with respect to Δ_{n+1}) :

(13) $$\mathbf{A}^n\ \mathbf{C}_f^{n+1} = \mathbf{B}^n\mathbf{C}_f^{n} \ - \ \mathbf{CM}\ (\mathbf{C}_a^{n+1} - \mathbf{C}_a^{n}) \ - \Delta_{n+1}\mathbf{F}^{n+0.5},$$

where

$$\mathbf{C}_a^{n+1} - \mathbf{C}_a^{n} = \gamma_{n+1}(\varphi(\mathbf{C}_f^{n}) - \mathbf{C}_a^{n}\ ) \quad \text{or} \quad \mathbf{C}_a^{n+1} - \mathbf{C}_a^{n} = \Delta_{n+1}\varphi_{ir}(\mathbf{C}_f^{n}),$$

(corresponding to (10.a)) (corresponding to (10.b))

$$\mathbf{A}^n = \mathbf{CM}^* + 0.5\Delta_{n+1}\mathbf{ST}_n^* , \quad \mathbf{B}^n = \mathbf{CM}^* - 0.5\Delta_{n+1}\mathbf{ST}_n^* ,$$

$$\gamma_{n+1} = \Delta_{n+1}\gamma/(1 + 0.5\Delta_{n+1}\gamma) .$$

The matrix $\mathbf{ST}_n^*$ can be computed according to the FE approximation

$$(14) \qquad \sum_e \bar{D}^e \int_{\mathcal{V}^e} \mathbf{grad}\, N_i \mathbf{grad}\, N_j dv ,$$

where $\bar{D}^e$ is obtained by averaging the nodal values of $\bar{D}$ in the element with number e ; N_i are the element shape functions and $\mathcal{V}^e$ is the element domain.

The following criterion for the time step choice is proposed to improve numerical solution accuracy :

$$(15) \qquad \| C_f^{n+1} - C_f^n - 2C_f^{n+0.5} \| = M_f \Delta_{n+1}^2 < \varepsilon \bar{c} , \quad M_f = \text{const.},$$

and

$$\| C_a^{n+1} - C_a^n - 2C_a^{n+0.5} \| = M_a \Delta_{n+1}^2 < \varepsilon \bar{c} , \quad M_a = \text{const.}$$

(only in case of a reversible reaction)

where: $C_f^{n+0.5}$, $C_a^{n+0.5}$ are obtained from (13) under the same known vectors C_f^n, C_a^n and a time step equal to $\Delta_{n+1}/2$;

$\| C_k \| = \max_k | C_k |$, k=1, ..., M , C being a vector in the space induced by N_i;

ε is a reasonable accuracy ;

$\bar{c}$ is a characteristic value of the species concentration (as an initial, boundary or equilibrium one) usualy used for introducing dimensionless concentrations so that $\| C_f \| \leq \bar{c}$.

The proposed difference method is investigated under the physical correctness conditions concerning problems (1) - (4) :

- c_f, c_a, $D(c_f)$ (or $D(x, y, z)$), $\varphi(c_f)$, Ψ_i, i = 1,2,3, c_f^o, c_a^o are positive and bounded functions;
- $\varphi_{ir}(c_f)$ is a bounded function.

The numerical solutions for C_f^{n+1} and C_a^{n+1} can be evaluated from (13) as follows:

(16.a) $$C_f^{n+1} = \tilde{B}_n C_f^n - \gamma_{n+1} D_n(\varphi(C_f^n) - C_a^n) + \Delta_{n+1} A_n^{-1} F^{n+1},$$

(16.b) $$C_f^{n+1} = \tilde{B}_n C_f^n - \Delta_{n+1} D_n \varphi_{ir}(C_f^n) + \Delta_{n+1} A_n^{-1} F^{n+1},$$

(17.a) $$C_a^{n+1} = (1-\gamma_{n+1}) C_a^n + \gamma_{n+1} \varphi(C_f^n),$$

(17.b) $$C_a^{n+1} = C_a^n + \Delta_{n+1} \varphi_{ir}(C_f^n),$$

where $\tilde{B}_k = A_k^{-1} B_k$, $D_k = A_k^{-1} CM$.

The necessary and sufficient condition for the physical correctness of the numerical solution in case of a reversible reaction is derived from (17.a) as follows :

(18) $$\gamma_{n+1} \leq 1 \quad \text{or} \quad \Delta_{n+1} \leq 2/\gamma .$$

After serial subtitutions of C_f^k and C_a^k in (16.a,b) and (17.a,b) for k = n, n-1, ..., 1 C_f^{n+1} and C_a^{n+1} are expressed in terms of the initial and boundary conditions in the following implicite form:

(19.a) $$C_f^{n+1} = \prod_{k=1}^{n} \tilde{B}_k C_f^o - \sum_{k=0}^{n} G_k D_k \varphi(C_f^k) + L C_a^o + \tilde{F},$$

(19.b) $$C_f^{n+1} = \prod_{k=1}^{n} \tilde{B}_k C_f^o - \sum_{k=0}^{n} \Delta_{k+1} \prod_{m=k+1}^{n} \tilde{B}_m D_k \varphi_{ir}(C_f^k) + \tilde{F},$$

(20.a) $$C_a^{n+1} = \prod_{k=1}^{n} (1-\gamma_k) C_a^o + \sum_{k=0}^{n} \prod_{m=k+1}^{n} (1-\gamma_{m+1}) \gamma_{k+1} \varphi(C_f^k),$$

(20.b) $$C_a^{n+1} = C_a^o + \sum_{k=0}^{n} \Delta_{k+1} \varphi_{ir}(C_f^k),$$

where $$F = \sum_{k=0}^{n} \Delta_{k+1} \prod_{m=k}^{n-1} \tilde{B}_{m+1} A_k^{-1} F^{k+0.5}$$

and G_k, L represent linear matrix forms including products of γ_k, $1 - \gamma_k$, $\tilde{B}_k$ and D_k , k = 1, 2, ... n .

As φ and φ_{ir} are bounded functions we could yield :

(21) $$\| \varphi(C_f)\| \le M_1 \| C_f \|, \quad \| \varphi_{ir} \| \le M_2 \| C_f \| ,$$

$$M_1 = \text{const.}, \quad M_2 = \text{const.}$$

The sufficient conditions for the time scheme stability are derived from (18)-(21) as follows [14] :

(22) $$\| \tilde{B}_n \|_1 < 1 , \quad \| D_n \|_1 < 1 , \quad n = 1,...,N ,$$

(23.a) $$\gamma_{n+1} M_1^n < 1 , \quad n = 1,...,N ,$$

(23.b) $$\Delta_{n+1} M_2^n < 1 , \quad n = 1,...,N ,$$

where M_i^n is equal to M_i from (21) for $C_f = C_f^n$, $i = 1, 2$ and $\| . \|_1$ denotes the matrix norm induced by the vector one $\| . \|$ defined in (15).

These conditions can be presented in the form:

(24) $$\left\| \left(I + 0.5\Delta_{n+1} CM^{*-1} ST_n^* \right)^{-1} \left(I - 0.5\Delta_{n+1} CM^{*-1} ST_n^* \right) \right\|_1 < 1 ,$$

(25) $$\left\| \left(I + 0.5\Delta_{n+1} CM^{*-1} ST_n^* \right)^{-1} \right\|_1 < 1 ,$$

(26.a) $$M_1^n < 1 , \Delta_{n+1} \le 2/\gamma \quad \text{or} \quad M_1^n \ge 1 , \Delta_{n+1} \le 1 /\gamma(M_1^n - 0.5),$$

(26.b) $$\Delta_{n+1} < 1 / M_2^n .$$

The matrix $CM^{*-1} ST_n^*$ is positive definite as the values of D are positive and bounded. Hence (24) and (25) are satisfied (according to the Kelog's lemma [14] and the FE matrices properties) and we can yield the proposed difference method is absolutely stable with respect to the boundary conditions. The sufficient conditions for the initial stability are expressed in (26.a,b). Their general form has to be precised for a given function φ or φ_{ir} .

3. Numerical algorithm

A FORTRAN program "DS-2" for solving two-dimentional problems of the type (1-4) is created on the basis of an algorithm, including the following main steps:

- Input of Data for:
1. Geometrical and model parameters;
2. Simplex elements characteristics used for FE Domain Discretisation;

3. Initial and boundary conditions;
4. Acurracy ε.
- Computing the Arrays for FE Domain Discretisation of (1-4) [13];
- Cyclic Operations in Time for n = 0, 1, ..., N :

A.0. Initial choice of the time step according to (26.a,b) :

$$\Delta_{n+1} = \Delta^{o}_{n+1} \ ;$$

A.I. Aditional Choice of the time step by using criterion (15) and the operations from A.II. on the intervals $[t_n, t_n + \Delta^{i}_{n+1}]$ and $[t_n, t_n + \Delta^{i}_{n+1}/2]$, for i = 0, 1..., k so that $\Delta^{i+1}_{n+1} = \Delta^{i}_{n+1}/2$, i.e the procedure until (15) satisfied for i = k and the choice is done as follows :

$$\Delta_{n+1} = \Delta^{k}_{n+1} \ ;$$

A.II. Application of the difference scheme (13) in int.

$$[t_n, \Delta^{o}_{n+1}]$$

discretised by $t_i = i\,\Delta^{k}_{n+1}$, i = 1, ..., 2^k.

1. Computing $\mathbf{A}^n$ and the wright side vector in (13) operating with the corresponding to the FE matrices (symmetric and of special sparse type) one-dimensional arrays [13];
2. Solution of the obtained linear equations system by the Gaussian or Least Square method [14], modified in accordance to the used one-dimensional array for $\mathbf{A}^n$;

A.III. Numerical evaluation of $M(t_{n+1})$ following the FE approximation:

$$M(t) = \sum_{e} (\bar{c}^{(e)}_{f} + \bar{c}^{(e)}_{a}) S^{(e)} \ ,$$

where: $M(t)$ is the total amount of the considered species in the domain (both free to diffuse and adsorbed); $\bar{c}^{(e)}_{f}$ and $\bar{c}^{(e)}_{a}$ are obtained by averaging the nodal values in the element with number e and $S^{(e)}$ is the area of the same element (in case of a two-dimensional domain).

4. Numerical examples

The proposed numerical approach for solving (1-4) is tested by the boundary problem :

$$\frac{\partial c_f}{\partial t} = D\left[\frac{\partial^2 c_f}{\partial x^2} + \frac{\partial^2 c_f}{\partial y^2}\right] - \frac{\partial c_a}{\partial t} \quad \text{in } \mathcal{V} = \{0 \le x < a;\ 0 \le y \le a/6\} \quad \text{for } t > 0 \tag{27}$$

$$\frac{\partial c_a}{\partial t} = \eta(R c_f - c_a) \quad \text{in } \mathcal{V} \text{ for } t > 0 \ , \ R = \text{const.} \tag{28}$$

(29) $$c_f = c^o \quad \text{for } x = a\ ,\ 0 \le y \le b\ ,\ t > 0\ ,$$

(30) $$c_f = c_a = 0 \quad \text{in } \mathcal{V} \text{ for } t = 0\ .$$

This example is chosen because of the availability of analytical results for a corresponding problem concerning diffusion and first order reversible reaction in a plane sheet [12]. These results calculated for different values of the dimensionless parameters R and $\eta a^2/D$ represent the total species mass in half the sheet reffered to its finile equilibrium value M_{eq} versus a dimensionless time parameter ($Dt/(R+1)a^2$ and ηt). The corresponding numerical results are obtained by the programme "DS-2" discretising the domain $\mathcal{V}$ with 12 triangle elements. The initial time step choice is done under the derived from (26) conditions :

(31) $$\Delta_n \le 2/\eta \quad \text{for R} \le 1 \quad \text{and} \quad \Delta_n \le 1/\eta(\text{R- 0.5}) \quad \text{for R} > 1,$$

Using criterion (15) for $\varepsilon = 0.02$ and $\bar{c} = (R+1)\bar{c}_f$, (c_f is the equilibrium value of c_f) a very good correspondance between the numerical and the analitical results for M / M_{eq} is obtained (Fig. 1-3).

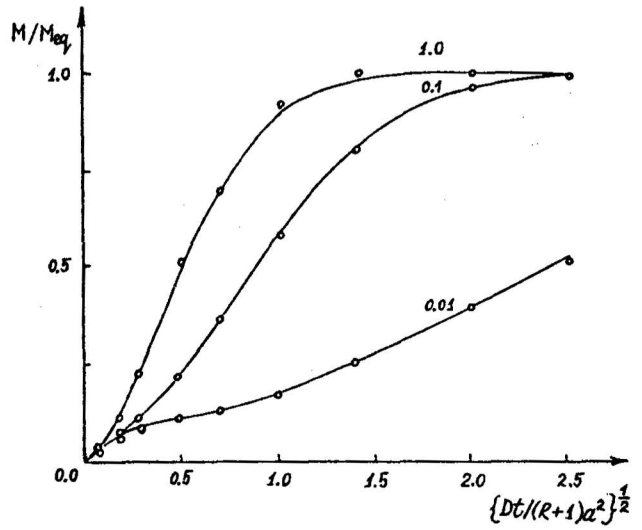

Fig.1. Numerical (open circles) and analytical (solid line) results when $R=10$. Numbers on curves are values of $\eta a^2/D$.

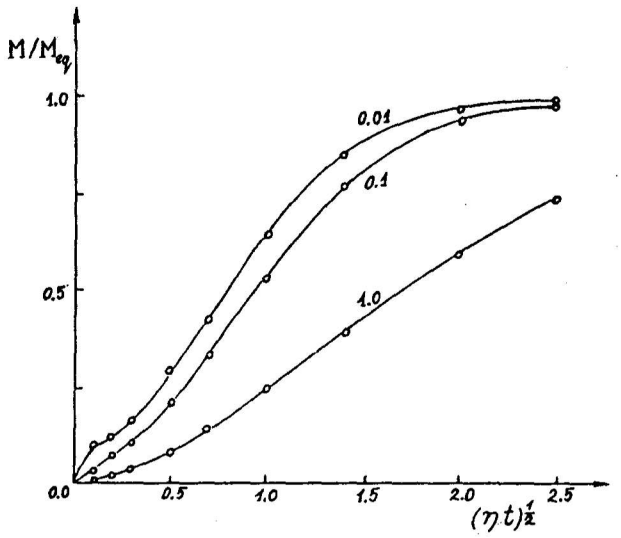

Fig.2. Numerical (open circles) and analytical (solid line) results when $R=10$. Numbers on curves are values of $\eta a^2/D$.

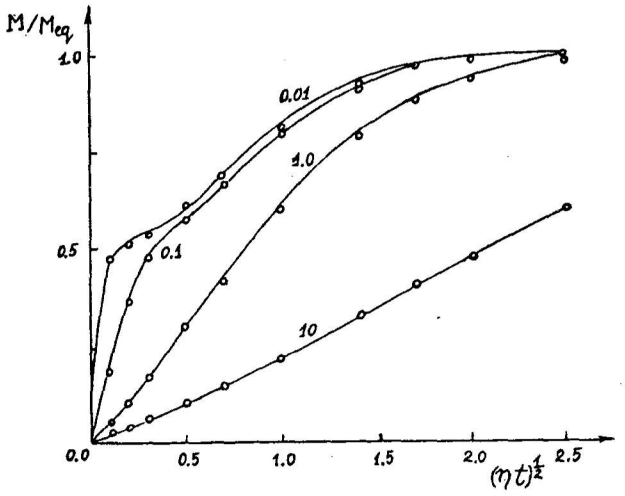

Fig.3. Numerical (open circles) and analytical (solid line) results when $R=1$. Numbers on curves are values of $\eta a^2/D$

5. Conclusion

A numerical approach for solving problems of the class (1-4) is developed using a FE domain approximation and a time difference method. The stability of the proposed hybrid scheme is investigated under the physical correctness conditions.

A general algorithm for two-dimensional problems of the considered type is constructed. Numerical examples for diffusion and first order reaction are provided by a FORTRAN programme. The obtained numerical results are in a very good correspondance with the available analytical ones when reaction and diffusion rate parameters are compareble values ($\eta a^2/D \in [0.01, 10]$ in Fig.1-3) i.e. a simultaneous diffusion and sorption is realised.

The proposed algorithm will be applied to some nonlinear problems in our further studies.

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