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MODELLING OF THE SIMULTANEOUS CONVECTION-DIFFUSION PROCESS THROUGH POROUS MEDIA WITH PERCOLATIVE-FRACTAL CHARACTER AT PRESENCE OF ANOMALOUS DIFFUSION

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Abstract: *Soil contamination with organic pollutants is one of the most serious environmental problems that can cause very serious threats to population and the environment. Therefore, the both experimental-, and modelling type investigation of such very complex-type transport processes are, and will be of crucial importance in the future, too. In agreement with the recent most advanced simulation methods, in the present work all results are realized on the base of the extended irreversible thermodynamics. A novel-type analytical solution is proposed for simultaneous convection-diffusion processes taking place through porous media. It is shown that the Riccati-type ordinary differential equation, frequently applied at modelling of the simultaneous convection-diffusion type processes, may be interpreted in a more general manner, as it has been done. The new modelling results are compared to the earlier analytical solutions and their relevance for accurate future modelling of such types of drying processes is also discussed. The completely novel-type solution of the problem indicated is realized in Lagrangian representation of continuum mechanics by extensive use of the MAPLE symbolic computer algebra system.*

Keywords: *Non-equilibrium thermodynamics; convection flow; anomalous diffusion; computational fluid dynamics*

INTRODUCTION

It is known, that in the contemporary theories of coupled transport processes through porous media methods of both non-equilibrium thermodynamics [1] and many ones from the confident, well-established results of the contemporary theories of critical phenomena relevant for percolative systems [2,3,4] should simultaneously be taken into account. Although many of these methods have also been applied in the contemporary modelling and simulation problems, there are further possibilities for their common new applications, to which our work is devoted, too. Particularly, the actual states of the different types of environmental problems require continuous improvement of the relevant complex transport models founded earlier. Besides, the direct determination of the corresponding characteristic material flow patterns is of crucial importance in this sense. Accordingly, in the present study, the newest confident methods of the non-equilibrium thermodynamics will be taken into account, as the most important ones.

METHODS

The basic PDE for modelling of the convection-diffusion problems is [5]:

$$\frac{\partial c}{\partial t}-\nabla\left(D(c)\nabla c\right)+\frac{dK}{dc}\cdot\frac{\partial c}{\partial z}=0, \tag{1}$$

where c(r,t) denotes the concentration distribution function, D(c,T) is the thermodynamically state-dependent diffusion coefficient, K(c) is the concentration-dependent hydraulic conductivity coefficient and z-axis corresponds to the direction of the gravitational acceleration. The general solution of the basic problem for a large class of convection - type transport processes through porous media can be suitably explained by the sums [5]:

$$c(\zeta)=a_0+\sum_{i=1}^{q}\left(a_i\cdot\omega^i+b_i\cdot\omega^{-i}\right),$$
$$a_0,a_i,b_i=\text{const.},\left(1\le i\le q\right),q\in\square \tag{2}$$

and it is explained by use of D'Alembert-type independent variables $\zeta:=x-v\cdot t$ (with a constant value "v" of the convection flow velocity). The physical meaning of the formula (2) is, that it gives analytical solution of the basic convection-diffusion equation (1) in the form of multiple travelling waves. Furthermore, simultaneous presence of convection and e.g. diffusion may also lead to appearance of wave-type transfer processes e.g. [6], it is also necessary to model drying processes from this point of view, too. Together with convection, the presence of anomalous diffusion [1,2], characteristic for genuine percolative-fractal systems is also taken into account in this study.

RESULTS AND DISCUSSION

The functions of the separate modes entering (2), must obey the Riccati-type ODE:

$$\frac{d\omega}{d\zeta}=\omega^2+k, \tag{3}$$

with "k" as a parameter depending on the actual experimental conditions [8]. The solutions of this basic convection-diffusion problem may be even of solitonic type. In order to realize our modelling work, we specify the eq. (3) as follows:

$$\omega'=\omega^2+k\rightarrow\omega'=\omega^2+\sum_m a_m(p)\zeta^m, \tag{4}$$

i.e. the coefficient *k* has been replaced here by $\sum_m a_m(p)\cdot\zeta^m$, where the series expansion coefficients are also assumed to be of stochastic character, due to the genuine percolative-fractal character of the dried bulk porous material to be observed at mesoscopic level [7]. Then, it is necessary to extend the calculation method applied, in order to open possibility for including further terms beyond the "dominant term" into the general modelling procedure we are developing, i.e. by

$$\frac{d^2\omega}{d\zeta^2}-a_n(p)\cdot\zeta^n\cdot\omega(\zeta)=a_r(p)\cdot\zeta^r. \tag{5}$$

Therefore, we may directly apply the well-known basic general formula for solving the relevant inhomogeneous second-order ODE (6), and by this way we obtained (using [8]):

$$\omega(\zeta)=C_1\sqrt{\zeta}\cdot J_{\frac{1}{n+2}}(\xi)+C_2\sqrt{\zeta}\cdot N_{\frac{1}{n+2}}(\xi)+$$
$$+\zeta^{\frac{1}{2}}\cdot J_{\frac{1}{n+2}}(\xi)\times\int\frac{(-1)\cdot a_r(p)\cdot\zeta^r\cdot N_{\frac{1}{n+2}}(\xi)d\zeta}{J_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}N_{\frac{1}{n+2}}(\xi)\right]'-N_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}J_{\frac{1}{n+2}}(\xi)\right]'} \tag{6}$$
$$+\zeta^{\frac{1}{2}}\cdot N_{\frac{1}{n+2}}(\xi)\times\int\frac{a_r(p)\cdot\zeta^r\cdot J_{\frac{1}{n+2}}(\xi)d\zeta}{J_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}N_{\frac{1}{2}}(\xi)\right]'-N_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}J(\xi)\right]'},$$

where a new independent variable defined by $\xi:=\dfrac{2\sqrt{-a_n(p)}}{(n+2)\cdot\zeta^{-\left(\frac{n}{2}+1\right)}}$ has been applied. Then, the whole procedure applied here may be continued by taking into account gradually further terms from (4), having „less-dominant" character compared to the previous ones. In order to present our own new modelling results in this area (based on [8]), which already belong to the Extended Irreversible Thermodynamics (EIT), we will here firstly recall the crucial generalization of the basic linear parabolic-type PDE describing the diffusion processes (and corresponding to the choice q = 2 in the relevant expression given below):

$$\frac{\partial c}{\partial t}=D\cdot\frac{\partial^2}{\partial x^2}c^{q-1}(x,t)\Rightarrow c(x,t)=t^{-\frac{1}{q}}\cdot f\left(\xi=x\cdot t^{-\frac{1}{q}}\right). \tag{7}$$

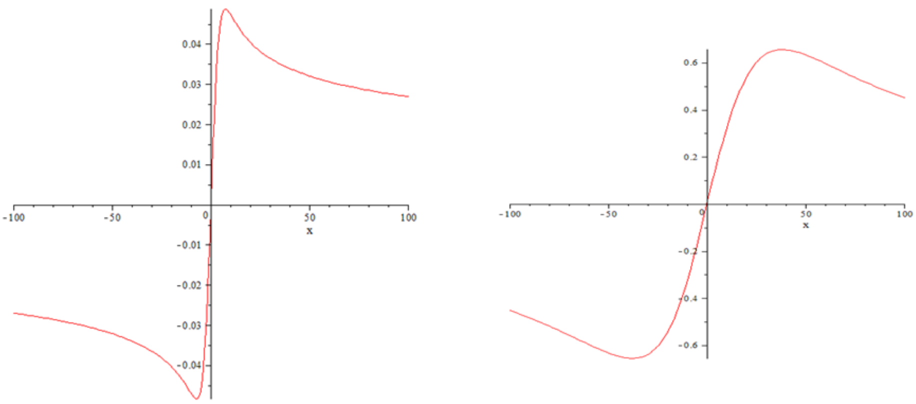
Then, the following two basic types can be recognized distinguished [1]:
Superdiffusion:

$$q\,\mathrm{f}\;2\Rightarrow f(\xi)=B\left(A^2-\xi^2\right)^{\frac{1}{q-2}},A=A(q),B=B(q), \tag{8a}$$

and subdiffusion:

$$q\,\mathrm{p}\;2\Rightarrow f(\xi)=B\left(A^2+\xi^2\right)^{\frac{1}{2-q}},A=A(q),B=B(q). \tag{8b}$$

In these new distribution function expressions the novel-type functions A = A(q), B = B(q) have also been introduced, in order to give mathematically correct modifications of the initial, classical-type distribution functions applicable in the case of the anomalous diffusion processes, too. Then, the following graphical presentations can be assigned to the e.g. supperdiffusive-type solution (9) for different values of finite-time moments (denoted in (9) by t_f) (Figure. 1(a-b)):



(a) (b)

Figure (2) Curvature characteristics of the superdiffusion solution functions represented for two different time moments t_f (in relative units)

CONCLUSIONS

In the present study a novel-type general method has been described for modelling of the simultaneous convection-diffusion processes taking place in bulk porous media. The relevance of the Riccati-type ordinary differential equation is accepted as a crucial mathematical background necessary for modelling of such types of complex transport processes. According to this novel-type algorithm for accurate modelling of the simultaneous convection-diffusion processes through bulk porous media, the possible problems appearing because of the inclusion of more than the first dominant convective term into the linearized Riccati's ordinary differential equation are also eliminated. Having solved this basic problem, we turned to incorporating of the relatively recently developed method of anomalous diffusion processes of the solution formulae and obtained completely new concentration distribution function expressions, which are of very promising and widespread applicable mathematical tools.

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