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A MODELLING OF THE COUPLED TRANSPORT PROCESSES THROUGH POROUS MEDIA AT PRESENCE OF ANOMALOUS DIFFUSION

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Abstract

The mathematical modelling of various types of coupled transfer processes plays nowadays a role of continuously increasing importance for understanding problems related to global energetic supply and dynamics of energetic systems in order to make them sustainable. Such methods are based on principles of the contemporary non-equilibrium thermodynamics, and are continuously re-examined and improved. In the present study, we will demonstrate a novel-type solution of the problem of coupled heat-, and mass transfer processes taking place through porous media, since this basic-type transport problem has countless number of applications ranging from e.g. modelling and simulation of drying processes till fundamental research calculations in the extended irreversible thermodynamics. The crucial novelty in our modelling method is the following one: it will be assumed, that the heat transfer may be described - as earlier – by a simple extension of the initial Fourier-type partial differential equation, while in the case of the diffusion, instead of the earlier usually applied Fick-type equations, the generalized version of its, able to describe anomalous diffusion processes must be incorporated into the initial coupled system of the relevant partial differential equations. Finally, following an earlier our own modelling method, we have solved this coupled system of partial differential equations by the usually applied operational calculation methods and have incorporated the effect of the anomalous diffusion effects, too. It was assumed, that the manifestations of the concentration changes due to anomalous diffusion are of second-order magnitude, but even under this assumption they influenced the final solution form of the problem very significantly.

Keywords*: thermodynamics, anomalous diffusion, environmental transport processes*

1. INTRODUCTION

It is known, that the contemporary theories of coupled transport phenomena through porous media require simultaneous application of methods of both non-equilibrium thermodynamics and many ones from the confident, well-established results of the contemporary theories of critical phenomena relevant for percolative systems [1-4]. Although the attempts to apply these two powerful physical theories in a common, hybridized form (in order to characterize the conductivity and coupling coefficients by their stochastic state-dependence – with particular care to their “crossover” behaviour, i.e. in the vicinities of critical points relevant for percolative phase transitions) has given us [3-4] some valuable results, this program is far from being completed.

Some recent very detailed modelling studies about applications of laser light – induced wave propagation treated the separate heat transfer (described by hyperbolic-type PDEs [5]) only, but not the simultaneous coupled heat and mass transfer in this sense. Therefore, this topic even nowadays represents a completely open research domain, despite of the above cited founding results, from which there are also some ones, existing for decades, too.

Firstly, we recall here a frequently used system of PDEs for mathematical modelling of drying processes (which represent an archetype of coupled transport processes) e.g. [6]:

$$\begin{aligned}\frac{\partial M}{\partial t} &= \nabla^2 a_{11} M + \nabla^2 a_{12} T + \nabla^2 a_{13} P,\\ \frac{\partial T}{\partial t} &= \nabla^2 a_{21} M + \nabla^2 a_{22} T + \nabla^2 a_{23} P,\\ \frac{\partial P}{\partial t} &= \nabla^2 a_{31} M + \nabla^2 a_{32} T + \nabla^2 a_{33} P,\end{aligned} \tag{1}$$

where M denotes the moisture content, T the temperature and P the pressure. The system of PDEs describing the coupled heat and mass transfer through capillary-porous bodies is usually based on the application of the zone picture, i.e. it is assumed, that the whole porous bulk may be divided into thin enough layers (the so-called zones) inside which the conductivity and coupling coefficients (incorporated into matrix elements a_{ij}) have constant values.

Moreover, the system of equations (1), as well as its simplified variants, is usually written in “criterial” form, i.e. the time t is to be understood as the Fourier-criterion ($t \rightarrow \frac{a_T t}{l^2}$, where a_T denotes the heat conductivity coefficient of the mixture and l is the characteristic length of the body being dried).

The relevant systems of coupled PDEs derived from (1) have been studied extensively in the literature of transport processes and permanently represent a very active research object from the point of view of modelling of such phenomena e.g. [6]. Another, frequently applied simplified version of (1) is [7]:

$$\begin{aligned}\frac{\partial c}{\partial t} &= D\nabla^2 c + K\nabla^2 T,\\ \frac{\partial T}{\partial t} &= E\nabla^2 T + L\nabla c,\end{aligned} \tag{2}$$

where c denotes now the concentration and T the temperature, D is the diffusion-, and E is the heat conduction coefficient. From the remaining coupling constants K is related to thermodiffusion (i.e. Soret-effect), and L to the heat amount carried by diffusion (i.e. Dufour-effect). Firstly, it will be assumed here, that in this coupled system of PDEs all coefficients are of constant value.

THE METHOD APPLIED

In this sub-section we will summarize briefly some essential mathematical features of the anomalous diffusion following [7], since at the end of the 13th Chapter of this well-known monograph about contemporary thermodynamics, the basic information about this active research area are presented concisely. Accordingly, the solution (at initial conditions described by Dirac’s delta-functions) of the generalized variant $\frac{\partial c}{\partial t} = D\frac{\partial^2}{\partial x^2} c^{q-1}\left(x,t\right),\left(q \in \check{}\ \right)$ of the diffusion equation has the following form:

$$c(x,t)=t^{-\frac{1}{q}}\cdot f\left(\xi=x\cdot t^{-\frac{1}{q}}\right), \tag{3}$$

resulting in $\left\langle(\Delta x)^2\right\rangle : t^{\frac{2}{q-1}}$ of the average value of the mean-square displacement, i.e. it generalizes the usual expression corresponding to the ordinary diffusion processes described by parabolic-type PDEs . Then, the following main particular cases are to be distinguished:

Normal diffusion:

$$q=2\Rightarrow f(\xi)=K\cdot e^{-\frac{\xi^2}{4D}},K=\text{const.}, \tag{4}$$

Superdiffusion:

$$q>2\Rightarrow f(\xi)=B\cdot\left(A^2-\xi^2\right)^{\frac{1}{q-2}},A=A(q),B=B(q), \tag{5}$$

Subdiffusion:

$$q<2\Rightarrow f(\xi)=B\cdot\left(A^2+\xi^2\right)^{\frac{1}{2-q}},A=A(q),B=B(q), \tag{6}$$

i.e. the possible values of the real-number parameter “q” are of decisive importance within frame of this modelling method. In order to demonstrate applicability of the above-sketched formalism, the limit situation of superdiffusion will be incorporated into solution formulae of the basic system (2).

Then, it was possible to calculate directly the relevant analytical solution formula of the superdiffusion transfer (by use of the MAPLE 10 system), given by the following expression [8-9] explained according to the Lagrangian representation [6] of continuum mechanics:

$$\begin{aligned}c_{\text{SupDiff}}(x,t_f)=\Bigg[&\frac{B\cdot\left(A^2\right)^{\frac{1}{q-2}}}{3A^2(q-3)(q-2)}\cdot F\left(\left[\frac{1}{2},-\frac{1}{q-2}\right],\left[\frac{3}{2}\right],-\frac{t_f^{-2/q}\cdot x^2}{A^2}\right)+\\&+\frac{2(q-3)x^2}{t_f^{3/q}}F\left(\left[\frac{q-3}{q-2},\frac{3}{2}\right]\left[\frac{5}{2}\right],-\frac{t_f^{-2/q}\cdot x^2}{A^2}\right)+6vxq\cdot F\left(\left[\frac{3}{2},-\frac{q}{2}\right],\left[\frac{5-q}{2}\right],-\frac{t_f^{-2/q}\cdot x^2}{A^2}\right)\Bigg],\end{aligned} \tag{7}$$

i.e. the results are explained by effective use of the hypergeometric special function $F([a,b],[c],x)$, and solution in the case of superdiffusion is less complicated, which fact is in complete agreement with the expected general experimental characteristics of the problem (because the convective flow contribution may in this case – in contrast to the convection – subdiffusion case - to suppress the superdiffusion contribution transfer in a much smaller amount, than it is characteristic in the case of subdiffusion).

The time parameter value t_f in (7) denotes the interval, during which the superdiffusive-type transfer of moisture has been observed in a given bulk porous material. In order to combine all these preliminary modelling results successfully, we will firstly apply here the extended version of (2), which – in agreement with WAT – can be written as:

$$\begin{aligned}\tau_1\frac{\partial^2 c}{\partial t^2}+\frac{\partial c}{\partial t}&=D\nabla^2 c+K\nabla^2 T,\\\tau_2\frac{\partial^2 T}{\partial t^2}+\frac{\partial T}{\partial t}&=E\nabla^2 T+L\nabla c,\end{aligned} \tag{8}$$

i.e. in the form of hyperbolic-type PDEs, instead of the usually applied coupled systems of parabolic-type PDEs. In agreement with our earlier result [4], it will be assumed here, that the relaxation time constant τ_1 relevant for moisture level changes is much more significant, than τ_2 corresponding to the temperature function.

Then, the general solution of the problem being discussed can be obtained as a solution of the following integro-differential equation of general character, under given initial-, and boundary conditions:

$$\tau_1 \frac{\partial^2 c(x,t)}{\partial t^2} + \frac{\partial c(x,t)}{\partial t} - D\frac{\partial c^{q-1}(x,t)}{\partial x^2} +$$
$$+ \frac{1}{4\sqrt{\pi} t^{3/2}} \cdot \frac{K}{E^{3/2}} \int_\Omega T_0(\xi)\left[1 - \frac{(x-\xi)^2}{2Et}\right] \cdot e^{-\frac{(x-\xi)^2}{4Et}} d\xi +$$
$$+ \frac{1}{4\sqrt{\pi} t} \cdot \frac{K}{E^{3/2}} \int_0^t \frac{1}{\sqrt{t-\eta}} \int_\Omega \frac{\partial^2 M(\xi,\eta)}{\partial \xi^2}\left[1 - \frac{(x-\xi)^2}{2Et}\right] \cdot e^{-\frac{(x-\xi)^2}{4Et}} d\xi d\eta = 0,$$

where, for the sake of simplicity only the „x" is used as a spatial coordinate.

Conclusion

In the present work the limit situations of anomalous diffusion processes are studied in the case, when thermodynamical cross-effects are also present in a given macroscopic dissipative continuum. It has been shown, that this newly proposed modelling method can be incorporated into the earlier, classical mathematical descriptions of the coupled heat and mass transfer processes taking place in bulk porous matter.

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