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Mathematical modeling of the simultaneous convection–anomalous diffusion processes in porous media

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ABSTRACT

After a brief overview of most important general features of the nonclassical diffusion on the base of the extended irreversible thermodynamics, the relevant mathematical formulae are incorporated into general formalism of the simultaneous convection–diffusion processes taking place in porous media. Then, using the simplest variant of the convection–diffusion equation, novel-type analytic solutions are derived for transport processes with both subdiffusion and superdiffusion characters in Lagrangian representation.

KEYWORDS

Anomalous diffusion; convection; drying; symbolic computation

Introduction

It is known that the contemporary theories of coupled transport phenomena through porous media require simultaneous application of methods of both nonequilibrium thermodynamics^[1] and many others from the confident, well-established results of the contemporary theories of critical phenomena relevant for percolative systems.^[2–4] Although the attempts to apply these two powerful physical theories in a common, hybridized form (to characterize the conductivity and coupling coefficients by their stochastic state dependence—with particular care to their “crossover” behavior, i.e., in the vicinities of critical points relevant for percolative phase transitions) has given us some valuable results,^[4,5] this program is far from being completed. Furthermore, since the genuine microscopic structure of the porous matter is adequately described not simply as a percolative system but rather than system of percolative fractal character, this latter fact should also be respected at accurate modeling procedures of all types of transport processes taking place in porous media. Since the mathematical modeling of convection–diffusion processes plays an important role in many other fundamental research and practical engineering transport process problems, elaboration of new and more accurate models for its represents a permanent task, whose complexity is reflected in the nonlinear character of the relevant ordinary differential equations (ODEs) and partial differential equations (PDEs) to be solved. Besides, at mathematical modeling of fast drying processes, the

usually applied mathematical formalism based on coupled parabolic type PDEs is unsuitable, since the classic descriptions of heat and mass conductivity processes are based on the Fick’s and Fourier’s law, which must be corrected for interpreting the experimental results emanating from use of laser light impulse technique.^[6] Besides, some earlier results in the literature^[7] also indicated that the theoretical and experimental re-examination of the role of cross-effects in the classic mathematical formalism of coupled transport processes may lead to a better agreement between simulations and measurement results in the case of unsteady drying processes. Our own earlier modeling method,^[8] where we applied coupled parabolic-type and hyperbolic-type PDEs and also the basic scaling relations relevant percolative systems, is also in agreement with this concept. In our relatively recent study, we have also demonstrated^[9] that a detailed symmetry analysis of the already existing formalism of coupled transport processes may lead to completely new types of oscillatory solutions of very general character (which have also been applied in plasma physics^[10]), and which do not suffer from the basic mathematical problem of the infinitely large propagation velocities, characteristic for solutions of separate parabolic type PDEs. Therefore, the classic wave approach of thermodynamics (WAT),^[11] as a most basic formalism of the extended irreversible thermodynamics, should have also been incorporated into accurate mathematical modeling methods of drying processes. Some recent and very

detailed modeling studies about applications of laser light-induced wave propagation^[12] treated only the separate heat transfer (described by hyperbolic-type PDEs), but not the simultaneous coupled heat and mass transfer in this sense. Therefore, this topic represents even nowadays a completely open research domain, despite of the above-cited well-known founding results.

Relevance of the convective flow at modeling of drying processes

Recent state of the art of mathematical modeling of drying processes at presence of convective flows

In this section, we will point out and discuss the relevance of the convection flow processes, playing also an important role in drying processes. First, the simultaneous presence of wave-type transfer processes and convection flow has not been examined in detail, although in the above-mentioned references (particularly in reference^[11]) the necessity of such approaches has also been emphasized. Second, since it is also known in the literature that simultaneous presence of convection and diffusion may also lead to the appearance of wave-type transfer processes,^[13] it is also necessary to model drying processes from this point of view. Therefore, in the present study, we will examine in detail this second limit situation in order to refine modeling of such types of transport phenomena. In the case of simultaneous convection and diffusion processes, the following PDE is to be applied, for example, see references^[14,15]:

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

where $c = c(\vec{r}, t)$ denotes the concentration distribution function to be determined, $D = D(c, T, \dots)$ is the (generally: thermodynamically state-dependent) diffusion coefficient, $K = K(c)$ is the concentration-dependent hydraulic conductivity coefficient, and z -axis corresponds to gravitational acceleration direction. Moreover, investigation of the convection-dominated transport processes through porous media led to the elaboration of some novel variants of discretization calculation methods, among which the so-called flow-line diffusion method^[15] seems to be a particularly promising one in future applications. The solutions of PDEs of type (1) may be sometimes even of solitonic type and therefore require the use of most effective methods developed within framework of the general theory of nonlinear ODEs and PDEs. As it is well known, the solitons may exist due to balance between

dispersion effects, which try to expand the initial localized wave packet, and the effects formally characterized by nonlinearities trying to localize it. After a detailed analysis of these opposite effects, Fan^[14] proposed a general method for solving nonlinear PDEs, according to which the linear term of highest order must be balanced with the nonlinear terms in the actual initial PDE to be solved. Then, if we represent the solution using the usual D'Alembert-type independent variable $\zeta = x - v_{co} \cdot t$ (with v_{co} as a constant velocity, i.e., we are dealing with traveling wave-type solutions^[13]) as $c = c(\zeta)$, its general form can be represented as:

$$c(\zeta) = a_0 + \sum_{i=1}^q (a_i \beta^i + b_i \beta^{-i}) \quad (2)$$

$$\beta = \beta(\zeta), \quad a_0, \quad a_i, \quad b_i = \text{const.}$$

where $q \in \mathbb{Z}^+$, and all of the component solution functions obey the Riccati-type ODE $(d\beta/d\zeta) = b + \beta^2$ with b as a parameter depending on the actual experimental conditions. As a novel element, together with convection, the presence of anomalous diffusion,^[16–18] characteristic for genuine percolative fractal systems, is also taken into account in the present work. Having discussed the basic general features of the simultaneous convection–diffusion processes taking place through porous media, we are now in position to apply the methods of the nonclassical diffusion theory,^[1,16–19] representing an essentially new improvement of the ordinary diffusion theory. Then, a refinement will be realized here through the application of theory of nonclassical diffusion, some essential points of which are presented concisely in the next section, together with a simple, but a new modeling method related to limit situations of the simultaneous presence of anomalous subdiffusion (or superdiffusion) process taking place through a porous medium and the convection flow. Therefore, the possible solutions of the evolution equation for the concentration $(\partial c/\partial t) + \vec{v} \cdot \nabla c = D \nabla^2 c$ (which is more general, than the usually applied Fick's equation, because it contains the convective term, too, e.g.,^[13,20] and may describe dispersion phenomena, too, according to which a wave packet of an arbitrary form can be represented^[13] as a superposition of harmonic waves; this fact was of decisive importance for preferring the substantial representation^[1,13] of continuum mechanics instead of the local one, which otherwise has been more frequently applied in this area) will be refined in the present work by taking into account characteristic features of the anomalous diffusion. Finally, we would like to point out that the usually applied technique of Riemann–Liouville operators,^[17,18] which is also of importance at detailed

modeling of anomalous diffusion phenomena, will not be used here, but instead we will apply another suitable mathematical formalism also elaborated within the frame of contemporary extended irreversible thermodynamics.

Incorporation of the anomalous diffusion formalism into modeling methods of simultaneous convection–diffusion processes

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

$$c(x,t) = t^{\frac{2}{q-1}} \cdot f\left(\xi = x \cdot t^{\frac{1}{q-1}}\right) \quad (3)$$

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

Normal diffusion:

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

Superdiffusion (faster than Fickian diffusion):

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

Subdiffusion (slower than Fickian diffusion):

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

where $A = A(q) = \text{const.}$, $B = B(q) = \text{const.}$, that is, the possible values of the real-number parameter q are of decisive importance from the point of view of the modeling of different types of diffusion processes. Since in the literature—at least according to our knowledge—the explicit functional forms of relations $A = A(q)$, $B = B(q)$ have not been discussed in detail, we will assign two pairs of constant values to them in this study.

Results

Finally, in this section, we will treat the simultaneous convection–anomalous diffusion processes in a simple,

but novel manner. Therefore, on the basis of well-known expression $\frac{dc}{dt} = \frac{\partial c}{\partial t} + v \cdot \nabla c$ for substantial time derivatives, we will present solutions for the both sub- and superdiffusion in the one-dimensional case and for a given, finite time interval. The superdiffusion case is of particular interest in the present study, because its basic feature (i.e., when the diffusion process is much faster than in the case of ordinary, simple diffusion) makes possible approach, according to which some basic features relevant for the usual, one-dimensional gas flow^[21] may also be exploited here. Accordingly, by direct use of the MAPLE computer algebra system,^[22] we arrive at:

$$\begin{aligned} & \frac{A^2(3-q)(q-2)}{B \cdot (A^2)^{1/(q-2)}} \cdot c_{\text{SubDiff}}(x,t) \\ &= -3 \cdot t^{-1/q} \cdot F\left(\left[\frac{1}{2}, \frac{-1}{q-2}\right], \left[\frac{3}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) A^2 q^2 \\ &+ 2 \cdot t^{\frac{q-3}{q}} x^2 q \cdot F\left(\left[\frac{q-3}{q-2}, \frac{3}{2}\right], \left[\frac{5}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) \\ &+ 6v \cdot t^{\frac{q-3}{q}} x q \cdot F\left(\left[\frac{3-q}{2}, \frac{q-3}{q-2}\right], \left[\frac{5-q}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) \\ &+ 15 \cdot t^{-1/q} \cdot F\left(\left[\frac{1}{2}, \frac{-1}{q-2}\right], \left[\frac{3}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) A^2 q + \\ &- 6 \cdot t^{-3/q} x^2 \cdot F\left(\left[\frac{q-3}{q-2}, \frac{3}{2}\right], \left[\frac{5}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) + \\ &- 18 \cdot t^{-1/q} \cdot F\left(\left[\frac{1}{2}, \frac{1}{q-2}\right], \left[\frac{3}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right). \end{aligned} \quad (7)$$

Similarly, it was also possible to calculate directly the relevant analytical solution formula of the superdiffusion transfer (again by the use of MAPLE 10 system), given by the following expression:

$$\begin{aligned} C_{\text{SupDiff}}(x,t) &= \left[\frac{B \cdot (A^2)^{\frac{1}{q-2}}}{3A^2(q-3)(q-2)} \right. \\ &\cdot F\left(\left[\frac{1}{2}, \frac{-1}{q-2}\right], \left[\frac{3}{2}\right], \frac{-t^{-2/q} \cdot x^2}{A^2}\right) + \frac{2(q-3)x^2}{t^{3/q}} \\ &F\left(\left[\frac{q-3}{q-2}, \frac{3}{2}\right], \left[\frac{5}{2}\right], \frac{-t^{-2/q} \cdot x^2}{A^2}\right) + 6vxq \cdot \\ &F\left(\left[\frac{3}{2}, \frac{-q}{2}\right], \left[\frac{5-q}{2}\right], \frac{t^{-2/q} \cdot x^2}{A^2}\right) \Big], \end{aligned} \quad (8)$$

i.e., in both cases the results are explained by effective use of the hypergeometric special function $F([a, b], [c], x)$, for example,^[22,23] 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

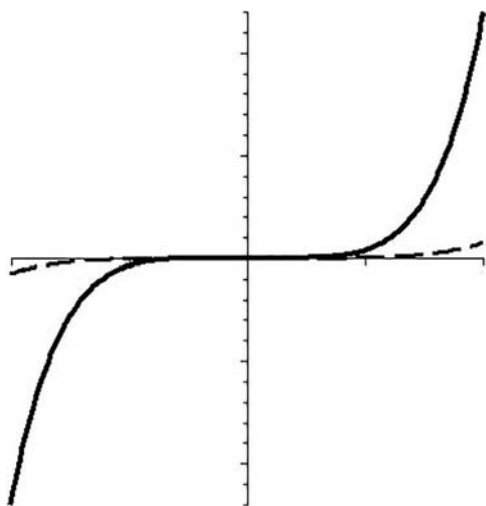


Figure 1. Concentration distribution curves of the simultaneous convection-anomalous superdiffusion transfer processes through porous bulk media (in relative units).

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 a characteristic in the case of subdiffusion). The diffusion exponent q was first taken to have value of 4 (in agreement with the basic requirements of the superdiffusion limit situation). Then, the relevant graphical representation above (in which—for the sake of simplicity—all quantities incorporated into coefficients of hypergeometric functions in (8) are assumed to have constant values including the time t and the convection velocity v) shows that at simultaneous convection and anomalous diffusion processes through porous media, which are in general case of percolative fractal character, novel-type moisture level distribution functions may be derived. This is illustrated in Fig. 1, where the two presented concentration distribution curves differ only in the values of the coefficients $A = A(q)$ and $B = B(q)$, respectively, which were taken to differ the two curves presented, while all the other quantities (except the spatial coordinate x , which is the independent variable according to the representation applied) are assumed to have constant values. (The constants A and B have double numerical values in the case of the dashed line—curve compared to the ones used at drawing of the continuous line—curve.)

Furthermore, the method proposed here by us may also be synthesized with the earlier, well-established methods about simultaneous convection and diffusion transfer processes through porous media.^[24]

Conclusion

In the present work, the limit situations of anomalous diffusion processes are studied in the case, when

convective flows are also present in a given macroscopic dissipative continuum. The Lagrangian representation of continuum mechanics is applied for both sub- and superdiffusion processes and completely novel-type formulae are derived directly by the use of MAPLE symbolic computer algebra system. Since the solution formulae are explained through the extended use of some basic-type special functions, results of this study must be developed in detail further to incorporate some earlier results of the topic and to contribute to some recent modeling results in convection–diffusion processes taking place in porous media and which could be of importance in future drying engineering practice. Among them, the detailed modeling of fast drying processes, induced by applying of, for example, laser radiation also represents a very promising future research area from this point of view, because some elements of the classical theory of propagation of shock waves might also be applied.

Nomenclature

A	numerical constant
a_0	numerical constant
a_i	numerical constant
B	numerical constant
b	numerical constant
b_i	numerical constant
c	concentration distribution function (kg/m ³)
D	diffusion coefficient (m ² /s)
F	hypergeometric-type special function
q	diffusion exponent
R	set of real numbers
T	temperature (K)
t	time (s)
v	velocity (m/s)
x	spatial coordinate (m)
Z	set of integer numbers
z	spatial coordinate (m)

Greek symbols

β	convection–diffusion mode
ζ	D'Alembert-type independent variable (m)
ξ	generalized propagation mode-type independent variable (m/s ^{1/q})

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