

Mathematical Modelling of Simultaneous Convection and Anomalous Diffusion Phenomena at Drying

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ABSTRACT. A new method for modelling of the simultaneous convection and diffusion processes through porous media is given. It is based on the extended tanh-method, leading to travelling wave-type solutions and requires application of a Riccati-type ordinary differential equation. It is shown, that this general method is in agreement with the classic descriptions of Rayleigh-type surface waves. A stochastic state-dependence is assigned to coefficients appearing in the Riccati-equation and its solutions obtained successfully reproduce the earlier basic results of the problem. Finally, the propagation of the moisture wave of nonlinear character through porous medium at simultaneous convection and anomalous diffusion is described in Lagrangian representation of the continuum mechanics.

KEYWORDS: Drying, convection, percolation, anomalous diffusion

1 Introduction

It is known, that the contemporary theories of coupled transport processes through porous media (including theoretical foundations of drying processes) require simultaneous application of methods of both continuum mechanics and many from the newest results of statistical mechanics e.g. (Tsimpanogiannis et al. 1999). Although the attempts to apply these two powerful physical theories in a common, hybridized form (in order to replace the thermodynamic state-dependence of 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 some promising results (Farkas et al. 2000, Mészáros et al. 2001, Mészáros et al. 2004, Mészáros and Bálint 2011), this programme 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 must also be taken into account at accurate modeling procedures of all types of transport processes taking place in porous media.

In the present work an attempt is given for creating a general solution method for modeling of the “wandering moisture level zone” phenomenon relevant for convective drying of bulk porous materials (Ayensu 2004). Namely, exchange of moisture takes place in a finite depth or layer in the drying zone, as the heated air takes up the moisture by convection and is cooled by evaporation. Using D’Alembert-type independent variables, the essence of the whole modeling problem may be reduced to exploitation of some basic invariance properties of a Riccati-type ordinary differential equation (ODE) emanating from the basic mathematical model of the convection-diffusion problem being studied (Fan 2000, Elwakil et al. 2004). As a novel element, together with convection, the presence of anomalous diffusion (Jou et al. 2001), characteristic for percolative-fractal systems is also taken into account in the second part of the present work. The recent modeling methods allow direct incorporation of advanced mathematical techniques (Atanacković et al. 2012) relevant for anomalous diffusion into existing transport models elaborated for simultaneous convection and diffusion taking place in porous media. Some characteristics of the model developed may be of importance at studies of the Bénard-Marangoni type convection phenomena (Zeytounian 1998, De Gennes et al. 2004), too.

Moreover, since mathematical modelling of the convection-diffusion processes plays an important role in many other fundamental research- and practical engineering transport process problems e.g. (Pascal 1993, Elwakil et al. 2004), elaboration of new and more accurate models for it represents a permanent task, whose complexity is reflected in the nonlinear character of the relevant ODEs and partial differential equations (PDEs) to be solved. In the case of simultaneous convection and diffusion processes the following PDE is to be applied:

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

where $c = c(\vec{r}, t)$ denotes the concentration distribution function to be determined, $D = D(c, T, \dots)$ is the (usually) thermodynamic state-dependent diffusion coefficient, $K = K(c)$ is the concentration-dependent hydraulic conductivity coefficient and z -axis corresponds to gravitational acceleration direction. In some of our previous studies about convective drying processes e.g. (Kirschner et al. 2004), we were faced with the necessity

of linearising of the initial PDE systems of nonlinear character related to convection flows. Moreover, investigation of the “convection-dominated” transport processes through porous media led to elaboration of some novel variants of discretization calculation methods, e.g. the flow-line diffusion method (Knabner and Angermann 2000) seems to be a particularly promising one.

The solutions of PDEs of type (1) may be sometimes even of solitonic type (Elwakil et al. 2004) and require application of the most effective methods developed within framework of the general theory of the nonlinear ODEs and PDEs, including soliton theory. 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 detailed analyses of these opposite effects Fan (Fan 2000) proposed a general method for solving effectively nonlinear PDEs, according to which the linear term of highest order must be balanced with the nonlinear terms in the initial PDE to be solved. Then, if we represent the solution by suitably chosen D'Alembert-type independent variables $\zeta = x - v_f \cdot t$ (with v_f as a constant velocity, i.e. we deal with travelling-wave type solutions), in the form of $c = c(\zeta)$, its general form can be written as (Fan 2000, Elwakil et al. 2004):

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

$$a_0, a_i, b_i = \text{const.}, 1 \leq i \leq q,$$

where $q \in \mathbb{Z}^+$, and the component solution functions obey the Riccati-type ODE $\frac{d\beta}{d\zeta} = b + \beta^2$ with „b” as a parameter depending on the actual experimental conditions. In the present study we will generalize these previously applied modelling methods by assuming stochastic state-dependence of the coefficients „b” instead of taking them as constants. After brief summary of main characteristics of the calculation method proposed by us (Mészáros et al. 2012), we turn to the general solution of the convection-diffusion problem using the general canonical form of the Riccati's ODE. In the case of the simplest description of the simultaneous convection-diffusion processes we have:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + v \frac{\partial c}{\partial x}. \quad (3)$$

The spreading out of the basic solution curve (i.e. dispersion) in the form of travelling waves can be assigned to the convection-diffusion equation (Eck et al. 2008), which will be applied here by change of the convection flow velocity direction with respect to (1). Equation (3) is able to reflect the most essential features of travelling waves with dispersive character. Namely, if we use the general solution form of travelling waves $c(x,t) = c_0 \cdot e^{i(kx - \omega t)}$ (c_0 as is the maximal value of the oscillating vector component) its direct substitution into (3) gives:

$$\omega = vk - iDk^2. \quad (4)$$

We may also state, that extensive application of the Riccati ODE at solving different types of travelling wave problems has its roots e.g. (Landau and Lifshitz 2000) in classic modelling methods leading to accurate descriptions of the Rayleigh-type surface gravitational waves. The above example may be directly generalized to the case of simultaneous convection and diffusion of several components, and the Lagrangian representation of continuum mechanics has proven to be particularly suitable from this point of view (Mészáros and Bálint, 2011).

2 Results and Discussion

Application of the Riccati-equation in the presence of inhomogeneous terms

We will use here the linearized variant of the Riccati ODE by specifying a function $h(\zeta) = \sum_m a_m p \cdot \zeta^m$ (instead of constants „b” in (2)), where the coefficients are of stochastic character, i.e. in the relation $a_m = a_m p$ the independent variable „p” will be defined as the *actual* percolation probability. The use of this stochastic state-dependence of series expansion coefficients is motivated by the methods applied by us (Farkas et al. 2000, Mészáros et al. 2001, Mészáros and Bálint, 2011), according to which the possible analytic solutions of the given macroscopic transport problem with (under given initial and boundary conditions) may be refined via *a posteriori* randomization on the base of scaling relations emanating from the theories of phase transitions taking place in percolative-, and percolative - fractal systems.

Let us assume firstly, that there is only one „dominant term” in the inhomogeneous term $h(\zeta)$. According to the solution method proposed in this paper, we modify here (following our own method presented in (Mészáros et al., 2012)) the Riccati’s ODE emanating from (2) as:

$$y' - y^2 - a_n p \cdot \zeta^n = 0. \quad (5)$$

(The variable $y = y(\zeta)$ is here naturally not identical with the simple independent variable y usually denoting a spatial coordinate). If we perform linearization of ODE (9), we have to solve the following second order ODE:

$$\frac{d^2 y}{d\zeta^2} + a_n p \cdot \zeta^n \cdot y = 0. \quad (6)$$

The solution of this ODE can also be obtained directly (again, by use of the MAPLE 10 system), and its final form is:

$$\begin{aligned} y(\zeta) = & C_1 \sqrt{\zeta} \cdot J_{\frac{1}{n+2}} \left(\frac{2\sqrt{a_n p} \cdot \zeta^{\frac{n}{2}+1}}{n+2} \right) + \\ & + C_2 \sqrt{\zeta} \cdot Y_{\frac{1}{n+2}} \left(\frac{2\sqrt{a_n p} \cdot \zeta^{\frac{n}{2}+1}}{n+2} \right), \quad (7) \\ & C_1, C_2 = \text{const.}, \end{aligned}$$

i.e. the final result is explained by Bessel-functions of the order $1/(n+2)$, which are of the first kind, and second kind respectively. The relevance of our solution can immediately be seen, if we compare (Figs 1-2) the graphical representation of the usually applied tanh-type solution (if $b < 0$), which is valid for ODE $\frac{d\beta}{d\zeta} = b + \beta^2$ emanating from (2) at $b = \text{const.}$ with solution (7) at low order.

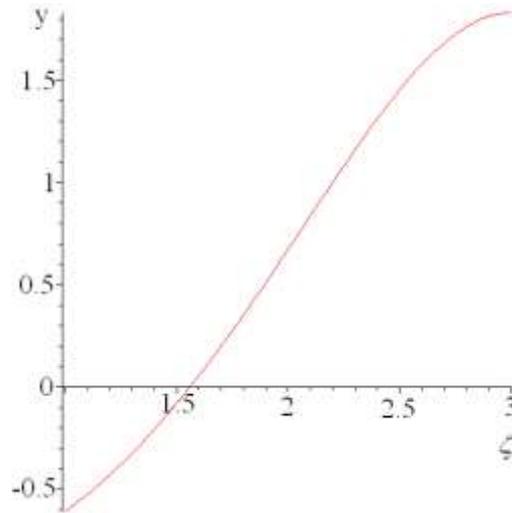


Fig. 1. Solution expressed by (7) for $n = 2$ (in relative units)

Since solutions of the Riccati - ODE emanating from (7) contains integration constants, we were here allowed to rescale the adequate coordinate systems and use relative units. This solution function may be considered as a refined variant of the basic *tanh*-solution, which has been applied (Fan 2000, Elwakil et al. 2004) till now.

A novel algorithm for modelling the convection- anomalous diffusion process problem through porous media

In the present section, we will treat the simultaneous convection-anomalous diffusion processes in a simple, but novel manner. Its essence is, that we will explain the concentration distribution function not in the usually applied Eulerian representation of continuum mechanics, but the Lagrangian picture will be applied here. Therefore, on the base of the relation $\frac{dc}{dt} = \frac{\partial c}{\partial t} + \vec{v} \cdot \nabla c$ for substantial time-derivatives (directly emanating from the general relationship $c = c(\vec{r}, t)$ e.g. (Jou et al., 2001)) we will have for the one-dimensional case and a given, finite time t_f (due to very complicated character of the subdiffusion concentration function, we present here the relevant formula of the superdiffusion only):

$$c_{\text{SupDiff}}(x, t_f) = \frac{B \cdot A^2 \frac{1}{q-2}}{3A^2 \frac{q-3}{q-2}} \left(\frac{3A^2 \frac{q^2-5q+6}{t_f^{1/q}}}{t_f^{1/q}} \right) + \left(F\left(\left[\frac{1}{2}, -\frac{1}{q-2}\right], \left[\frac{3}{2}, -\frac{t_f^{-2/q} \cdot x^2}{A^2}\right]\right) + \frac{2 \frac{q-3}{t_f^{3/q}} x^2}{t_f^{3/q}} F\left(\left[\frac{q-3}{q-2}, \left[\frac{5}{2}, -\frac{t_f^{-2/q} \cdot x^2}{A^2}\right]\right]\right) + 6vxq \cdot t_f^{\frac{q-3}{3}} F\left(\left[\frac{3}{2} - \frac{q}{2}, \frac{q-3}{q-2}\right], \left[\frac{5-q}{2}, -\frac{t_f^{-2/q} \cdot x^2}{A^2}\right]\right) \right) \quad (8)$$

i.e. the result is explained by effective use of the hypergeometric special function $F(a, b, c, x)$. The relevant graphical representations below illustrate, that at simultaneous convection and anomalous diffusion processes through porous media,

which are in general case of percolative-fractal character, completely novel-type moisture level distribution functions must be taken into account.

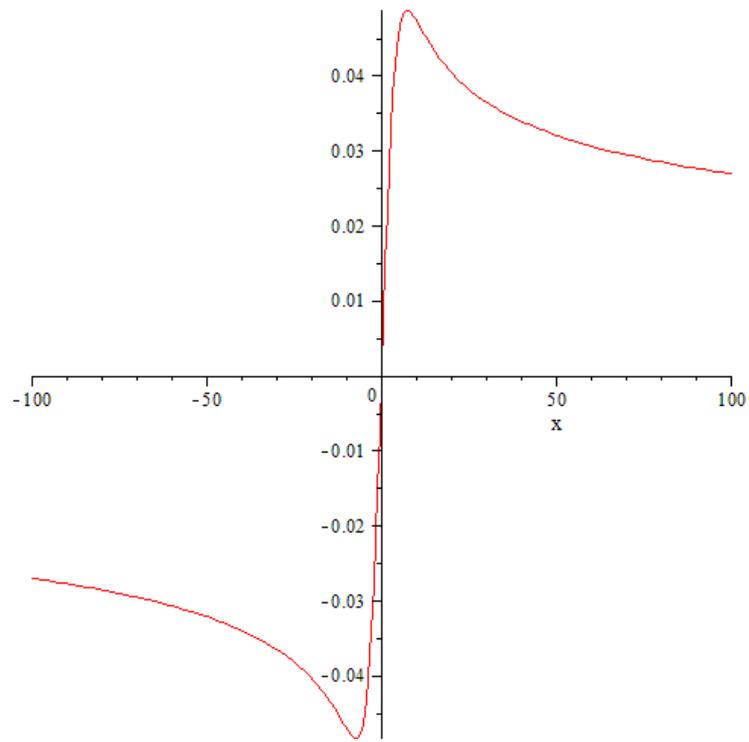


Fig.2. Concentration function at $t = 15$ (in relative units).

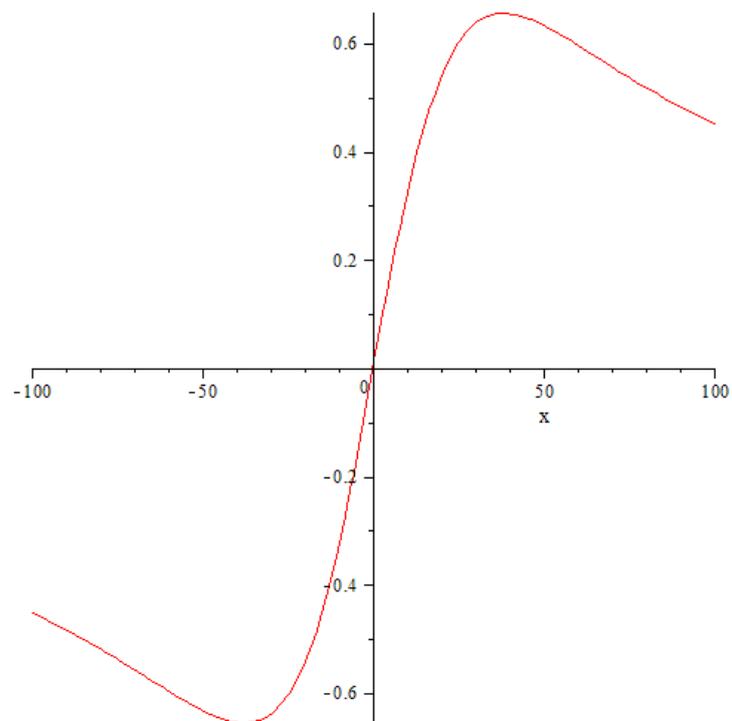


Fig.3. Concentration function at $t = 350$ (in relative units).

It can be immediately seen, that the solution has a clearly-visible shock-wave-like shape, characteristic for one-dimensional gas-flow phenomena e.g. (Landau and Lifshitz 2000). Besides, there is a clearly visible spreading out of the initial shape of the wave during time and the curvature characteristics of the shock-wave function is determined by concrete numerical values of the quantities A, B, v and q.

Appendix

In this Appendix we summarize briefly some essential mathematical features of the anomalous diffusion following Jou et al. (Jou et al., 2001), since at the end of the 13th Chapter (about non-classical diffusion) of this well-known monograph, the basic informations about this active research topic are summarized in a very suitable manner. Accordingly, the solution (at initial conditions expressed by Dirac's delta-functions) of the generalized variant $\frac{\partial c}{\partial t} = D \frac{\partial^2}{\partial x^2} c^{q-1}(x, t)$, $q \in \mathbb{R}$ of diffusion equation has a general-type solution in the form of :

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

resulting in $\langle \Delta x^2 \rangle \approx t^{\frac{2}{q-1}}$ of the average value of the mean-square displacement. Then, the following main particular cases are to be distinguished:

- Normal diffusion:

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

- Subdiffusion:

$$q > 2 \Rightarrow f(\xi) = B \cdot A^2 - \xi^2 \frac{1}{q-2}, A = A(q), B = B(q), \quad (\text{A},3)$$

- Superdiffusion:

$$q < 2 \Rightarrow f(\xi) = B \cdot A^2 + \xi^2 \frac{1}{2-q}, A = A(q), B = B(q). \quad (\text{A},4)$$

3 Conclusions

In the present work we solved the basic convection-diffusion method by fully exploiting the basic invariance properties of the Riccati ODE emanating from the general solution method of the problem initiated by Fan. As a novel element, the possible stochastic state-dependence of the series-expansion expression coefficients emanating on the right-hand side of this ODE are implicitly also taken into account. This study of the previously used mathematical models of the simultaneous convection and diffusion through porous media should lead to possibility of further refinements of the basic tanh-solution and effective comparisons with models taking explicitly into account the general percolative-fractal character of porous media.

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