Mathematical Modelling of Simultaneous Convection-Diffusion-Reaction Systems Taking Place in Porous Media

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***Abstract**: In the present work a novel modelling method is proposed for mathematical modelling of simultaneous convection-diffusion processes taking place in soil columns on the base of a simultaneous application of methods of the non-equilibrium thermodynamics and statistical mechanics of percolative-fractal systems. Firstly, the complete analytical solution of the basic convection-diffusion problem is presented at various types of boundary conditions and the relevant solution functions are stochastically refined a posteriori on the base of scaling relations relevant for describing of critical phenomena taking place in percolative-fractal systems at mesoscopic level. In this sense, some pecularities relevant for coupled transport processes in drying engineering problems and simulatenous convection-diffusion processes through porous media in general sense are discussed in detail. Besides, the presence and crucial role of the Riccati-type differential equation is indicated in cases of the simultaneous convection-diffusion processes taking place in porous media. The results obtained in this way are compared with experimental results emanating from our measurements concerning changes of the moisture level- and temperature distribution functions in soil columns. Then, the simplest possible case of a two-component diffusion is discussed in detail, where the final solution form is expressed by use of the Lommel-type special functions (till now widely used in plasma physics only in sense of the mathematical modelling of transport processes, which can be treated within framework of the non-equilibrium thermodynamics and classical physical kinteics) on the base of a simple symmetry assumption about direct flow-, and cross-flow diffusion coefficients. Finally, some possible future research activity areas from the point of view the most general type convection-diffusion processes supplemented by simultaneous chemical reactions are also indicated.*

***Keywords:** convection-diffusion processes, extended irreversible thermodynamics, percolative-fractal systems*

1 Introduction

It is well-known nowadays, that experimental investigation and mathematical modelling of various types of (generally: coupled) transport processes according to the non-equilibrium thermodynamics represents crucial part of many engineering and fundamental complex research problems, including e.g. simulation of energy dispersal processes on global scale [1]. It may also be stated, that due to its relevance from the point of view of environment, this research area will be of crucial importance in future, too. From many mathematical aspects of this very important research domain we will emphasize here from the beginning the necessity of applying of variational methods of the non-equilibrium thermodynamics e.g. [2], (usually called extended irreversible thermodynamics in its most up-to-date form [3], [4]) and general theory of percolative-fractal systems (i.e. the most general mathematical discipline relevant for description of the bulk porous matter at mesoscopic level) [5]. Both these disciplines are well-elaborated ones, supplemented by very effective mathematical methods, but their simultaneous, *common* application in a hybridized form is still far from being completed, despite of the fact, that it could be very useful in the future engineering applications of very different type. Therefore, in the present study we will try to demonstrate further methods and possibilities for realizing of this programme, basing our present modelling work on our, own previous research results [6-9].

2 A Direct Generalization of the Formalism of Coupled Transport Processes

In the present section we will recall concisely the essence of the generalization method of the coupled transport processes of different type tensorial orders on the base of our relatively recent study [10]. Accordingly, the thermodynamic cross-effects are of crucial importance at eliminating of the problem of infinitely large heat or mass transfer velocities emanating from the usual solutions of the separate, linear parabolic type partial differential equations usually applied within frame of the formalism of the classical irreversible thermodynamics, e.g. [2].

2.1 The Case of the Two-Component Diffusion

In order to present results of the calculation results emanating from the general method discussed above, we start here from the simplest possible case of simultaneous diffusion of a two-component system, whose constituents do not interact chemically. Accordingly, the following coupled system of parabolic-type partial differential equations (PDEs) must be solved:

$$\begin{aligned} \frac{\partial c_1}{\partial t} &= D_{11}\frac{\partial^2 c_1}{\partial x^2} + D_{12}\frac{\partial^2 c_2}{\partial x^2}, \\ \frac{\partial c_2}{\partial t} &= D_{21}\frac{\partial^2 c_1}{\partial x^2} + D_{22}\frac{\partial c_2}{\partial x^2}, \end{aligned} \tag{1}$$

where the thermodynamic cross-effects have also been taken into account.

2.1.1 Application of the Lommel-Type Special Functions

It is well-known, that in the simplified one-dimensional case, the concentration function can be written as (the series expansion coefficients k_n are constants, and the quantities λ_n denote the reciprocal values of the relevant n-th harmonics):

$$c(\vec{r},t) \equiv c(x,y,z,t) \to c(x,t) = \sum_n k_n c_n(x) \cdot e^{-\lambda_n t}. \qquad (2)$$

Substitution of the temperature and moisture level functions also represented in this series expansion form into system (1) gives the following equation:

$$\begin{aligned} &\sum_n k_{1n}\left[(D_{11}-D_{22}) \frac{d^2 c_{1n}(x)}{dx^2} + \lambda_{1n} \cdot c_{1n}(x) \right] \cdot e^{-\lambda_{1n} t} = \\ &= \sum_n k_{2n}\left[(D_{21}-D_{12}) \frac{d^2 c_{2n}(x)}{dx^2} + \lambda_{2n} \cdot c_{2n}(x) \right] \cdot e^{-\lambda_{2n} t}. \end{aligned} \qquad (3)$$

Since the equation system (3) is symmetric, we assumed [10], that the spatial harmonics of the same order of different relative concentration functions have the same functional form, i.e.

$$\frac{d^2 c_{1n}(x)}{dx^2} + \frac{\lambda_{1n}}{D_{11}-D_{22}} c_{1n}(x) = \frac{dc_{2n}(x)}{dx^2} + \frac{\lambda_{2n}}{D_{21}-D_{12}} c_{2n}(x) \propto \psi_n(x). \qquad (4)$$

It is obvious, that homogeneous parts of (4) represent the usual linear harmonic oscillator equations. For the sake of simplicity, we identify here the functions on their right-hand sights as simplest polynomials of the same order as the order of the relevant spatial harmonic is, i.e. $\psi_n(x) \propto x^n$. In general case, the functions on the right-hand side in the relations (4) will be presented as linear combinations of such elementary polynomials. Then, the ODEs (4) will have the following solution form [10]:

$$
\begin{aligned}
y(x) = {} & K_1 \cdot \cos\left(\sqrt{k}x\right) + K_2 \cdot \sin\left(\sqrt{k}x\right) - \frac{x^{1+n}}{k\sqrt{x\sqrt{k}}\left(3n+n^2+2\right)} \times \\
& \left[-\frac{1}{\left(x\sqrt{k}\right)^n}(n+2)(n+1)\cos\left(x\sqrt{k}\right) \times \right. \\
& \times \left(x^{1+n}\sqrt{k}\cos\left(x\sqrt{k}\right) - x^n \sin\left(x\sqrt{k}\right) LommelS1(n+\frac{1}{2},\frac{1}{2},x\sqrt{k}) \right) + \\
& + \frac{1}{\left(x\sqrt{k}\right)^n}(n+2) LommelS1\left(n+\frac{3}{2},\frac{1}{2},x\sqrt{k}\right) \\
& \left(x^{1+n}\sqrt{k}\sin\left(x\sqrt{k}\right)\cos\left(x\sqrt{k}\right) - x^n + x^n\cos^2\left(x\sqrt{k}\right)\right) + \\
& + x^{1+n}\sqrt{k}\left(\frac{n}{\left(x\sqrt{k}\right)^n}(n+2)(\cos(x\sqrt{k}-1)^2 LommelS1(n+\frac{1}{2},\frac{3}{2},x\sqrt{k}) \right) - \\
& \left. - \cos\left(x\sqrt{k}\right)\sin\left(x\sqrt{k}\right)\left(\sqrt{x\sqrt{k}} + (n+1)\frac{1+n}{\left(x\sqrt{k}\right)^n} LommelS1\left(n+\frac{3}{2},\frac{3}{2},x\sqrt{k}\right)\right)\right],
\end{aligned} \tag{5}
$$

i.e. this calculation gave us an analytical result explained by the so-called Lommel-type special functions. This type of special functions had played an important role in plasma physics, too [10].

3 Modelling of the Simultaneous Convection-Diffusion Processes Taking Place in Porous Media

In the present section the crucial role of the Riccati-type ordinary differential equations will be discussed in detail for the case of simultaneous convection-diffusion processes together with indications concerning possible future applications of its matrix form.

3.1 Relevance of the Riccati-Type ODE at Mathematical Modelling of Simultaneous Convection-Diffusion Processes

As it has been emphasized above, since the mathematical modelling of the simultaneous convection-diffusion processes is of importance from the point of view of both fundamental researches and solving of engineering problems, too [6], [11] developing of new and more accurate models of this problem represents a permanent task, whose complexity is reflected in the nonlinear character of the

ODEs and PDEs corresponding to it, to be solved e.g. [12]. The basic PDE for the convection-diffusion problem is e.g. [13]:

$$\frac{\partial c}{\partial t}-\nabla\cdot\left(D(c)\nabla c\right)+\frac{dK}{dc}\cdot\frac{\partial c}{\partial z}=0, \tag{6}$$

where $c=c(\vec{r},t)$ denotes the concentration distribution function to be determined, $D=D(c,T,...)$ is the usually: thermodynamic state-dependent diffusion coefficient and $K=K(c)$ is the concentration-dependent hydraulic conductivity coefficient and z-axis corresponds to the direction of the gravitational acceleration. The solutions of PDEs of type (6) may be sometimes even of solitonic type [13]. Such 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. By a detailed analysis of these opposite effects, Fan [12] proposed a general method for solving the relevant nonlinear PDEs. Accordingly, 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 solutions by use of D'Alembert-type independent variables: $\zeta=x-v\cdot t(v=const.)\Rightarrow c=c(\zeta)$, in the case of convection-diffusion problems, their general form will be:

$$\begin{aligned}&c(\zeta)=a_0+\sum_{i=1}^{q}\left(a_i\omega^i+b_i\omega^{-i}\right),\omega=\omega(\zeta),\\&a_0,a_i,b_i=const.,(1\le i\le q),\end{aligned} \tag{7}$$

where $q\in\Re^+$ and the component solution functions obey the Riccati-type ODE $\frac{d\omega}{d\zeta}=\kappa+\omega^2$ with parameter „κ" depending on the experimental conditions.

3.1.1 Refinement and Formalization of the Earlier Known, Basic Results

Firstly, in the present sub-section we will present a novel-type solution of the Riccati's ODE discussed previously using some very elementary facts about the relevance and possible influence of the percolative-fractal character of the bulk porous matter, inside which simultaneous convection-diffusion processes are taking place. Then, in order to solve the Riccati – ODE (related to (7)) the following form of its will be applied:

$$\omega'-\omega^2-\sum_m a_m(p)\zeta^m=0, \tag{8}$$

i.e. we intend to develop a refined modelling method, since the genuine convection - diffusion processes through porous media (e.g. through soil columns) are always sensitive to the underlying percolative-fractal character of matter at mesoscopic level. We use here the linearized variant of the Riccati's ODE (8) by specifying $h(\zeta)=\sum_m a_m(p)\cdot\zeta^m$, where the coefficients are of stochastic character, i.e. in $a_n = a_n(p)$ the independent variable *„p"* will be defined as the actual percolation probability. For the sake of simplicity we will assume firstly, that there is only one „dominant term" in this expression, i.e.:

$$\omega' - \omega^2 - a_n(p)\cdot\zeta^n = 0. \qquad (9)$$

In this case, the solution of the Riccati-type ODE is (as well as in the case of [5], we used the MAPLE computer algebra system [14]):

$$\omega = \frac{C\left[\phi(\zeta)\cdot J_{\frac{n+3}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right) - J_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right)\right]}{\zeta\left[CJ_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right) + N_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right)\right]} + \frac{C\left[\phi(\zeta)\cdot N_{\frac{n+3}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right) - N_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right)\right]}{\zeta\left[CJ_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right) + N_{\frac{1}{n+2}}\left(\frac{2\phi(\zeta)}{n+2}\right)\right]}, \qquad (11)$$

(i.e. the general form characteristic for the projective linear groups [15] can also be directly recognized in this solution form, too) where:

$$\phi(\zeta) \equiv \sqrt{a_n(p)}\cdot\zeta^{\frac{n}{2}+1}, \qquad (12)$$

and C is an integration constant, while $J_k(\zeta)$ and $N_k(\zeta)$ both denote the Bessel-functions of k-th order, which are of the first kind, and second kind respectively. It is obvious, that the basic invariance property (A1-A3) of the Riccati ODE is reflected in the form of the solution (11), too. Then, by linearizing the ODE (10), we have to solve the following second order ODE:

$$\frac{d^2\omega}{d\zeta^2} - a_n(p)\cdot\zeta^n\cdot\omega(\zeta) = 0. \qquad (13)$$

The solution of this ODE can be obtained directly (again, we used the MAPLE system [14]), and its final form is more concise compared to (11)):

$$\omega(\zeta) = C_1\sqrt{\zeta}\cdot J_{\frac{1}{n+2}}\left(\frac{2\sqrt{-a_n(p)}\cdot\zeta^{\frac{n}{2}+1}}{n+2}\right) + C_2\sqrt{\zeta}\cdot N_{\frac{1}{n+2}}\left(\frac{2\sqrt{-a_n(p)}\zeta^{\frac{n}{2}+1}}{n+2}\right) \qquad (14)$$

($C_1, C_2 = const.$), i.e. the final result is explained by Bessel-functions of the order $\frac{1}{n+2}$ (which are again of the first- and second kind, respectively), and presented graphically on Fig. 1.:

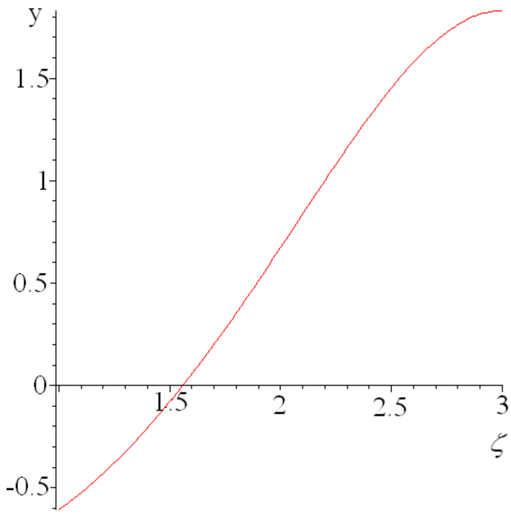

Fig. 1
Solution expressed by (14) for n = 2 (in relative units)

Despite of its different convexity character, this solution is not in contradiction to the basic tanh-type solution proposed in the study [12], but represents a more general and refined variant of its.

3.1.2 Introduction of a Novel-Type Modelling Algorithm

Then, having solved this basic problem, we are in position to refine the results explained by (14), by including further terms except the dominant one (i.e. in the sense of the relation (9)), i.e. we must solve the second-order ODE:

$$\frac{d^2\omega}{d\zeta^2} - a_n(p)\cdot\zeta^n\cdot\omega(\zeta) = a_r(p)\cdot\zeta^r, \tag{15}$$

where the right-hand side may be considered, as the "next dominant" term from $h(\zeta) = \sum_m a_m(p)\cdot\zeta^m$. It must be emphasized here, that this choice is also allowed, because the well-elaborated algorithms concerning solutions of infinite series of integrable Riccati-type ODEs [16-17], [18] are built up on the base of formulae, which contain arbitrary functions, too [18]. Therefore, having solved the "basic homogeneous problem" (13), we may directly apply the well-known basic general formula (based on the Lagrange's method of variation of constants) for solution of the relevant inhomogeneous second-order ODE (15), i.e. we have:

$$\omega(\zeta)=C_1\sqrt{\zeta}\cdot J_{\frac{1}{n+2}}(\xi)+C_2\sqrt{\zeta}\cdot N_{\frac{1}{n+2}}(\xi)+$$
$$+\zeta^{\frac{1}{2}}\cdot J_{\frac{1}{n+2}}(\xi)\times\int\frac{(-1)\cdot a_r(p)\cdot\zeta^r\cdot\zeta^{\frac{1}{2}}N_{\frac{1}{n+2}}(\xi)d\zeta}{\zeta^{\frac{1}{2}}J_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}N_{\frac{1}{n+2}}(\xi)\right]'-\zeta^{\frac{1}{2}}N_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}J_{\frac{1}{n+2}}(\xi)\right]'} \tag{16}$$
$$+\zeta^{\frac{1}{2}}\cdot N_{\frac{1}{n+2}}(\xi)\times\int\frac{a_r(p)\cdot\zeta^r\cdot\zeta^{\frac{1}{2}}J_{\frac{1}{n+2}}(\xi)d\zeta}{\zeta^{\frac{1}{2}}J_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}N_{\frac{1}{2}}(\xi)\right]'-\zeta^{\frac{1}{2}}N_{\frac{1}{n+2}}(\xi)\left[\zeta^{\frac{1}{2}}J(\xi)\right]'},$$

where a new variable defined by $\xi:=\frac{2\sqrt{-a_n(p)}}{(n+2)\cdot\zeta^{-\left(\frac{n}{2}+1\right)}}$ has also been applied.

4 Conclusions

In the present work an attempt is given for a general symmetry treatment of the simultaneous convection-diffusion phenomena taking place in porous media from a unique point of view. It is demonstrated, that further detailed applications of the Riccati-type equations should play a crucial role in the future symmetry analyses of these very general type dissipative structures. Besides, since the investigation of the most diverse types of convection-diffusion processes [19-20] even recently represent an active research area, it may be expected, that detailed applications of analytical solutions (realized by extensive use of the most advanced computer algebra systems) of such very complex transport problems may lead to important new results from the point of view of completely novel-type engineering applications, too. Moreover, by simultaneous applications of the results treated separately about coupled chemical reaction-diffusion systems and convection-diffusion processes, crucial new results can be derived from the point of view of studies of simultaneous convection-diffusion-chemical reaction non-equilibrium thermodynamic systems in a unique manner.

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6 References

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