Chin. Phys. B Vol. 20, No. 11 (2011) 110507

Transient transport processes in deformable porous media*

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(Received 28 March 2011; revised manuscript received 12 August 2011)

The basic partial differential equations relevant for convection-diffusion and convection-diffusion-wave phenomena are presented and solved analytically by using the MAPLE symbolic computer algebra system. The possible general nonlinear character of the constitutive equation of the convection-discussion process is replaced by a direct posteriori stochastic refinement of its solution represented for Dirichlet-type boundary conditions. A thermodynamic analysis is performed for connecting the relaxation time constants and Jacobi-determinants of deformations at transient transport processes. Finally, a new procedure for general description of coupled transport processes on the basis of the formalism originally developed for convection-free phenomena is presented by matrix analysis methods in the Fourier space.

Keywords: convection, binary mixtures, relaxation time, matrix polynomials

PACS: 05.70.Ln, 47.56+r, 02.10.Yn **DOI:** 10.1088/1674-1056/20/11/110507

1. Introduction

As shown by the extended irreversible thermodynamics (EIT),[1] the classical transport equations (i.e. Fick's relation for diffusion, Fourier's formula for heat conduction and Newton's one for viscous flow) are not always able to give an adequate description of the heat and mass transfer phenomena in many systems. The main reason of it is that they are implying infinitely large propagation velocities, which is incompatible with the basic principles of physics. In addition, investigation of the transfer processes called anomalous diffusion phenomena[2] nowadays plays a role of increasing importance in many areas of theoretical investigation and mathematical modeling of transport processes, and this concept is expected to develop into genuine thermodynamic theory of transport processes through porous media. However, even within the frame of the classical irreversible thermodynamics (CIT), it is still possible to obtain valuable new results, particularly in detailed studies of the thermodynamic cross-effects and different formalisms related to the wave theories of thermodynamics.[1] In the present work, we take into account the unsuitable character of the formalisms based on the application of separate parabolic type partial differential equations (PDEs). The problem of the infinitely large propagation velocities is usually resolved by introducing the nonzero relaxation time constants[3−5] to ensure presence of inertial phenomena[6] in transport processes. The systems which are characterized by long relaxation times are superconductors, low temperature heat and electric conductors, and particularly the polymeric fluids.[1] Polymer solutions represent particularly important examples of systems, where non-Fickian diffusion processes are taking place and among them, coating of substrates via deposition and subsequent drying of such solutions play a particularly important role in the relevant engineering practice. Serious experimental investigations of these systems[7] contributed to further understanding of the thermodynamic cross-effects, particularly thermodiffusion. The importance and further perspectives of the topic are generally also illustrated via detailed studies of percolation of the liquids through porous media by Onsager-type equations, which allowed even some fundamentally novel type applications of the corresponding tools of the physical kinetics, too.[8]

In general, investigation of convection processes through porous media also represents a very wide and dynamically developing research area from the same point of view. In order to illustrate the complex character of this field, we mention here some typical examples (without pretensions to completeness) of convective drying of porous media,[9] convection of multicomponent fluids through thermogravitational

*Project support by the Hungarian-German Foundation MÖB-DAAD (Grant No. P-MÖB/843).
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columns[10] and convection in colloidal suspensions.[11] We think it is particularly important in the present study that some of the newest theoretical and modeling results from the field of convective drying of shrinking media[12] are applications of convection-diffusion models in the case of binary liquids. The examination of the concept of frame-indifference in the case of viscoelastic media is also of interest for decades,[1] since it is acceptable only in the cases that the inertial effects are not significant.[13] Moreover, the use of the effective solution method leads to multiple travelling wave solution of the nonlinear PDEs[14] after its application to general type of convection-diffusion equations[15] resulted in understanding of different travelling wave types of transport processes in porous media. Among them, the solitary wave type solution is also allowed and it is one of the most interesting ones. The same circle of convection-diffusion problems has also been investigated by powerful methods of the Painlevé theory[16] developed for general analysis of nonlinear ordinary differential equations (ODEs) and nonlinear PDEs playing a role of increasing importance in various branches of the contemporary physics.[17]

The relevant forthcoming calculations will be mainly performed according to the linear approximation of the CIT. In order to give as general description of such problems as possible, description of deformation phenomena will also be incorporated into mathematical formalism applied in this paper. A convenient description of the transport problems characterized by shrinkage can be given in Lagrangian representation. This representation is applied even in numerical calculations, particularly in the so-called flow-line-diffusion method.[18] To exploit its characteristics, we will also summarize in this work the balance equations related to the problem being investigated, on the basis of general formalism of the EIT in a unified simple, but novel manner.

2. Analytical solution and stochastic refinement of the convection-diffusion equation

Firstly, we present the solutions of the basic convection, diffusion PDE related to the case of constant flow velocity $\boldsymbol{v}$ and thermodynamically state-independent conductivity coefficients. This equation is written for the one-dimensional case, i.e., for the concentration function $u(x,t)$, where x denotes the spatial coordinate, and t is the time. For simultaneous convection and diffusion, we have

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + v\frac{\partial u}{\partial x}. \tag{1}$$

Here, D is the diffusion coefficient.

The (1)-type PDE has been studied profoundly many times in the literature.[19] We solve it directly by use of the MAPLE-10 (MAPLE, 2005)[20] symbolic computer algebra system, which has made it possible for novel types of solutions of some fundamental convection problems, too.[21,22] The solutions of the space- and time-dependent parts are respectively

$$F_1(x) = K_1 \cdot \mathrm{e}^{\frac{(-v+\sqrt{v^2+4KD})}{2D}x} + K_2 \cdot \mathrm{e}^{-\frac{(v+\sqrt{v^2+4KD})}{2D}x}, \quad F_2(t) \propto \mathrm{e}^{Kt}, \tag{2}$$

where K, K_1 and K_2 are integration constants. The coefficient of constant value equating the time-dependent exponential factor with $F_2(t)$ will be directly incorporated into K_1 and K_2. For the existence of solutions with exponentially decaying character in time, it must satisfy $K < 0$ if this constant is of real value. We recall the explicit form of the earlier solutions from Ref. [19], where the analytical solution of the PDE (1) is derived by using the Laplace transformation method. The author[19] investigated the convection-diffusion phenomena in two-phase systems and used the constitutive equations in the form of

$$J = vu - Du^m \frac{\partial u}{\partial x}\left|\frac{\partial u}{\partial x}\right|^{n-1}, \tag{3}$$

where m and n are adjustable dimensionless parameters. The nonlinear character of the diffusion terms has also been taken into account. After specifying a linear case with diffusion coefficients of identical values for both the constituents of the system being investigated and the initial and boundary conditions as $u(0,t) = u_0 = \text{const.}$, $t > 0$ and $u(x,0) = 0, x > 0$ (assuming $v = 1$ for the sake of simplicity), the final explicit solution derived by Pascal was expressed by the formula

$$\frac{u_0}{2}\left\{\mathrm{erfc}\left[\frac{1}{2\sqrt{D}}\left(\frac{x}{\sqrt{t}} - \sqrt{t}\right)\right] + \mathrm{e}^{x/D}\mathrm{erfc}\left[\frac{1}{2\sqrt{D}}\left(\frac{x}{\sqrt{t}} + \sqrt{t}\right)\right]\right\}, \tag{4}$$

where the dimensionless character of the independent variables, those of the concentration functions and the characteristic parameters of the system being investigated were used. Some nonlinear cases (i.e. those corresponding to $m \neq 0$, $n \neq 1$) have also been examined in detail in the same work at various initial

and boundary conditions. We think it is most important from this study that the convexity character of curves of the concentration distribution functions depends on the values of m and n, and we will compare it with Eq. (2) in the case of Dirichlet-type boundary conditions, which will be specialized below. Therefore, the nonlinear character of the convection-diffusion problem will be modeled in this paper via subsequent stochastic refinement of the general solution of Eq. (1).

In the boundary condition analysis for the PDE (1), we will assume again that the convection flow velocity is of constant value. Then, the Dirichlet-type boundary condition is assumed to be valid for a vertical column of finite height with c_0 being the initial value of the concentration on the top of a column, which we considered as an outer constraint of constant value. The solution (2) takes the particular form[23]

$$u\left(x,t\right)=u_0\cdot \mathrm{e}^{-\frac{2vx+v^2t}{4D}}. \tag{5}$$

Despite of its simplicity, this solution form may represent a useful new expression for examining the convection-diffusion processes, as it will be demonstrated below. To include the role of porous microstructure of the matter into our modelling procedure, we use some basic results of the contemporary percolation theory.[24,25] This theory has successfully been applied in refined mathematical modelling of drying processes, particularly in descriptions of invasion percolation and percolation front widths in general. It is also the merit of these modelling approaches that they take into account the fractal character of the invasion percolation processes, too.[26−29] Despite of these advanced applications of the percolation theory in solving the fundamental drying engineering problems, we will turn back to the basic results of the problem of roaming on percolation clusters also known as the labyrinthine ant problem.[30] Namely, for modelling percolation processes on nodes via Monte–Carlo simulations, Mitescu *et al.*[31] applied the formulae

$$\begin{aligned}
&\langle R^2\left(t\right)\rangle \approx R_\infty^2\left[1-C_>\cdot \mathrm{e}^{-t/\tau}\right],\quad p>p_\mathrm{c},\\
&\langle R^2\left(t\right)\rangle \approx D\left[1+C_<\cdot \mathrm{e}^{-t/\theta}\right],\quad p<p_\mathrm{c},\\
&C_>=\text{const.},\quad C_<=\text{const.}
\end{aligned} \tag{6}$$

for the mean-value of square of the time-dependent displacement $R(t)$ in the vicinity of the critical percolation probability p_c, i.e., for the values $\Delta p = |p-p_\mathrm{c}| \ll 1$ of the actual percolation probability p. Here, R_∞^2 is the limit value of $\langle R^2\left(t\right)\rangle$ for $p<p_\mathrm{c}$.

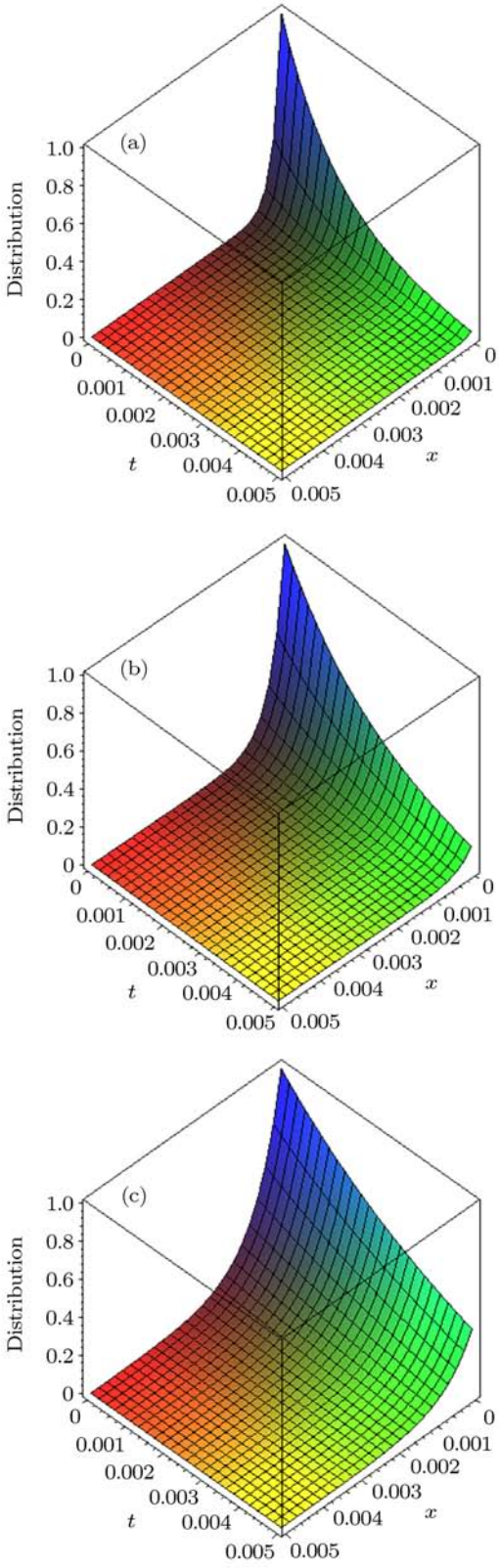


Fig. 1. (colour online) The concentration distribution function at $t_\mathrm{cond}=1,2$ of the critical index for (a) $\Delta p=0.0010$, (b) $\Delta p=0.0015$ and (c) $\Delta p=0.050$ of the percolation probability differences (in relative units).

Later, Straley [32] derived the following scaling rela-

tions relevant for the quantities in Eq. (6)

$$R^2_{\infty}(p) \propto \Delta p^{-2\nu+\beta}, \tau(p) \propto \Delta p^{-2\nu-t_{\rm cond}+\beta},$$
$$D(p) \propto \sigma_{\rm e}(p) \propto \Delta p^{t_{\rm cond}}, \theta(p) \propto \Delta p^{-2\nu-t_{\rm cond}+\beta}. \quad (7)$$

Here, ν denotes the critical exponent of the correlation length, β is the common symbol of the critical exponent of the order parameter at phase transitions and τ and θ are characteristic times, whose state-dependence is also obvious. Now, we use here a direct method for refinements of the modelling results obtained initially by linear approximation of the EIT, since this stochastic refinement of the general macroscopic results has shown sensitivity of the latters with respect to the actual percolative state of the capillary-porous system being investigated.[33−37] Therefore, a posteriori randomization of (5) will be performed on the basis of the value of the diffusion coefficient, explained by $D(p) \propto (\Delta p)^{t_{\rm cond}}$, where $t_{\rm cond}$ is a critical index of specific conductivity with allowed values of $t_{\rm cond} \in [1,2;1,6]$.

To compare our modelling results represented by these simple graphics, we recall here again the earlier cited results from Ref. [19]. We assume that the actual percolative state of the system may influence the shape of the concentration solution curves even more than it has been demonstrated in Fig. 1. Namely, in some earlier results of our study,[33−35] after analytic solution of a coupled system of parabolic- and hyperbolic- type PDEs relevant for general description of the simultaneous heat and mass transfer through porous matter, it has been shown that different values of the percolation probability may cause even a cross-over from a given convexity of the concentration distribution curve to the opposite one. In this respect, Fig. 5. in Pascal's article[19] is of particular importance for us, because it clearly demonstrates the influence of the nonlinearity parameter m on the shape of the concentration distribution function (at a given constant, the non-zero value of the convection flow velocity $\boldsymbol{v}$). This is in agreement with the solution curves presented in Fig. 1.

3. The balance equations and deformation phenomena in dissipative continua

In general case, the link between the substantial (Lagrange-) and local (Euler-) type balance equations can be demonstrated by the following relation,[38] which connects the relevant substantial and local derivatives

$$\rho\,\dot{a} = \frac{\partial \rho\, a}{\partial t} + \boldsymbol{\nabla}\cdot\rho\, a\, \boldsymbol{v}, \quad (8)$$

calculated per unit mass with $a = {\rm d}A/{\rm d}M$ as a specific extensive quantity calculated per unit mass. For the general theory of the convection-free coupled transport processes, i.e., for $\boldsymbol{v} = 0$, the relation (8) in which ρ denotes density is of basic importance. The concise description of derivation of the relevant system of coupled transport equations together with a novel method of its solution by Fourier transformation technique will be presented in Section 6. Then, since the source density function $\sigma_{\rm a}$ is equivalent in both Lagrangian and Eulerian representations, we may write

$$\rho\,\dot{a} + \boldsymbol{\nabla}\cdot\boldsymbol{J}_{\rm a} = \sigma_{\rm a} = \frac{\partial \rho\, a}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{J}^0_{\rm a}, \quad (9)$$

where $\boldsymbol{J}^0_{\rm a}$ is the local- and $\boldsymbol{J}_{\rm a}$ is the substantial flux. The second one from them (i.e. the one containing $\boldsymbol{J}^0_{\rm a}$), together with the continuity equation $\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot\rho\,\boldsymbol{v} = 0$ leads to

$$\frac{\partial a}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} a = -\frac{1}{\rho}\boldsymbol{\nabla}\cdot\boldsymbol{J}_{\rm a} + \frac{\sigma_{\rm a}}{\rho}, \quad (10)$$

which we introduce in the present paper as a characteristic hybrid representation, because the partial time derivatives used usually at Euler type descriptions are combined here with substantial fluxes $\boldsymbol{J}_{\rm a}$ relevant for the Lagrangian picture. Taking into account the deformations, we will have

$$\frac{\partial a}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} a = -\frac{|\boldsymbol{J}|_{\rm def}}{\rho_0}\boldsymbol{\nabla}\cdot\boldsymbol{J}_{\rm a} + \frac{\sigma_{\rm a}\,|\boldsymbol{J}|_{\rm def}}{\rho_0}, \quad (11)$$

where ρ_0 denotes the density of the continuum before deformation and $|\boldsymbol{J}|_{\rm def}$ is the Jacobi-determinant of the actual deformation, whose explicit form may take rather complicated form at solving of concrete, practical engineering problems. A detailed formalism from this point of view is developed in Ref. [12]. The connection between densities is in most general case given in Ref. [38] by the relationship $\rho_0 = \rho\,|\boldsymbol{J}|_{\rm def}$. The deformation phenomena may be incorporated into general formalism of the basic balance equations from the beginning, as it will be demonstrated below. In addition, only the simplest dissipative systems without chemical reactions will be examined here, i.e., $\sigma_{\rm a} = 0$ will be assumed to be valid.

4. Application of the Maxwell–Cattaneo–Vernotte theory

The modified constitutive equation which is used in this study is the classical Cattaneo–Vernotte

equation,[3–5] later generalized by Gyarmati to the case of coupled transport processes too.[39] In the case of simple heat conduction, this equation is

$$\boldsymbol{J} = -\lambda_T \boldsymbol{\nabla} T - \tau_T \frac{\partial \boldsymbol{J}}{\partial t}, \tag{12}$$

where the heat conduction coefficient λ_T and relaxation time constant τ_T are again both assumed to be of constant values, although in the formalism of Ref. [39], it is possible to explicitly take into account the eventual thermodynamic state-dependence of τ via relationship $\tau \to \tau_{ij} = -\sum_{l=1}^{F} L_{il} m_{lj}$, where F denotes the number of thermodynamic degrees of freedom of the system, L_{il} is the general element of the conductivity matrix and the non-positive matrix m_{lj} is the matrix of generalized inductivities in the entropy picture and coefficient of the kinetic part in the fully developed form of the general non-equilibrium entropy function, i.e.,

$$s = s_{\mathrm{eq}} + s_{kin} \equiv \sum_{l=1}^{F} \Gamma_l a_l + \frac{1}{2} \sum_{l,j=1}^{F} m_{lj} \boldsymbol{J}_l \cdot \boldsymbol{J}_j. \tag{13}$$

Here, in the equilibrium part of the entropy function, the quantities a and Γ-s are again the extensive and the intensive thermodynamic quantities which are both α-type (i.e. invariant) variables from the point of view of the time-reversal symmetry operation,[40] and $\boldsymbol{J}_l$-s denote the (components of the) fluxes in the same macroscopic dissipative continuum, i.e., they are building up β-type variables which change their sign to the opposite under the influence of the time-reversal symmetry operation. [40] An analogous equation is valid in the diffusion processes. Combination of these equations with the basic balance equations directly leads to coupled hyperbolic PDE system of the coupled heat and mass transfer. Illustrative applications are, for example, examination of the non-Fickian diffusion in binary mixtures at uniform temperature,[41] experimental investigation of fast and high-intensity drying processes by pulsed laser technique,[42] refinements[43] of the Luikov's system of equations by application of the EIT, numerical solution of the convection-diffusion equations based on Cattaneo's law by use of the finite element technique,[44] and detailed elaboration of the hyperbolic theory for advection-diffusion problems, etc.[45]

For purpose of general analysis in the forthcoming section, we also recall that the secondary viscosity coefficient ζ is related to the relaxation time constant τ by

$$\zeta = \frac{\tau \rho}{1 - \mathrm{i}\,\omega\tau} \left(c_{\mathrm{s}\infty}^2 - c_{\mathrm{se}}^2 \right), \tag{14}$$

where ω is the frequency of the periodic compression and expansion of adiabatic character, c_{se} is the sound velocity corresponding to an equilibrium state of the mixture and the velocity $c_{\mathrm{s}\infty}$ is related to the actual, non-equilibrium value of concentration of one of the mixture components. At derivation of Eq. (14) in the well-known monograph of Ref. [46], the authors start from the ODE $\frac{\mathrm{d}\xi}{\mathrm{d}t} = -\frac{\xi - \xi_0}{\tau}$, where by $\xi = \xi(t)$ an actual value of a quantity characterizing the thermodynamic state of the macroscopic dissipative continuum is denoted (e.g., relative concentration), ξ_0 is its equilibrium value, which in general case depends on density and temperature, and τ is the relaxation time constant. At solving of this ODE, we do not specify the periodic density changes of adiabatic character as it has been done in Ref. [46], but directly use its general integral

$$\xi(t) = \xi_0 + C_* \cdot \mathrm{e}^{-t/\tau}, \tag{15}$$

where C_* is an integration constant. Despite of its simplicity, the relation (12) will be of crucial importance in this paper.

5. Connection between deformations and relaxation time constants

To set up this connection, we study a two-component object, $\rho = \rho_1 + \rho_2$ denotes the density of the complete system, with ρ_1 and ρ_2 being the densities of its constituents. The choice $\rho_1/\rho = c_1 \to c$ and $\rho_2/\rho = c_2 \to 1 - c$ of relative concentrations is suitable[38,39] to identify the specific quantity a in Eqs. (8)–(11). Then, we will have

$$\rho_1 \boldsymbol{v}_1 = \boldsymbol{J}_1 + \rho_1 \boldsymbol{v}, \tag{16}$$

for the balance equation of the first component. The relevant constitutive equation will be modified according to the Maxwell–Cattaneo–Vernotte theory as

$$\boldsymbol{J}_1 = -\rho D \boldsymbol{\nabla} c \to \boldsymbol{J}_1 + \tau_1 \frac{\partial \boldsymbol{J}_1}{\partial t} = -\rho D \boldsymbol{\nabla} c, \tag{17}$$

where the relaxation time constant τ_1 is assumed to be a constant. The balance equation for the first constituent must also be applied as

$$\frac{\partial \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{J}_1^0 = 0 \tag{18}$$

at the local description of fluxes (local fluxes are again indicated by zero upper indices), or as

$$\frac{\partial \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{J}_1 + \boldsymbol{\nabla} \cdot \rho_1 \boldsymbol{v} = 0, \tag{19}$$

if we use the hybrid representation introduced at derivation of Eq. (11), where $\boldsymbol{v}$ is the macroscopic velocity of the convection flow. In the forthcoming calculations, we replace ρ_1 by ρc and so the direct combination of Eqs. (17)–(19) results in

$$\frac{\partial(\rho c)}{\partial t}+\tau_1\frac{\partial^2(\rho c)}{\partial t^2}+\boldsymbol{\nabla}\cdot(\rho c\boldsymbol{v})+\tau_1\frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot(\rho c\boldsymbol{v}) = \boldsymbol{\nabla}[\rho D\boldsymbol{\nabla}c], \tag{20}$$

i.e., the possible thermodynamic state-dependence of diffusion coefficient will be taken into account here. A well-known explicit expression for this concentration and temperature-dependence is the Arrhenius formula, $D=D(c,T)\propto \mathrm{e}^{-A_\mathrm{p}/c}\cdot\mathrm{e}^{-E_\mathrm{A}/RT}$, also applied in modeling of drying processes of the aqueous polymer solutions.[47] Here, A_p denotes a constant, E_A is the activation energy, and R is the universal gas constant. Therefore, in general case, the non-linear character of the actual transport process must be taken into account. Using again the continuity equation $\frac{\partial\rho}{\partial t}+\boldsymbol{\nabla}\cdot\rho\boldsymbol{v}=0$, we obtain

$$\left(\rho+\tau_1\frac{\partial\rho}{\partial t}\right)\cdot\frac{\mathrm{d}c}{\mathrm{d}t}+\rho\tau_1\frac{\partial^2 c}{\partial t^2} +\rho\tau_1\frac{\partial\boldsymbol{v}}{\partial t}\cdot\boldsymbol{\nabla}c+\rho\tau_1\boldsymbol{v}\frac{\partial}{\partial t}\boldsymbol{\nabla}c = \boldsymbol{\nabla}\cdot[\rho D\boldsymbol{\nabla}c] \tag{21}$$

from Eq. (20), and the relation $\frac{\mathrm{d}c}{\mathrm{d}t}=\frac{\partial c}{\partial t}+\boldsymbol{v}\cdot\boldsymbol{\nabla}c$ has also been used. Finally, from Eq. (21) by direct transformation to full Lagrangian frame of reference (accompanied by $\boldsymbol{v}=0$), we have

$$\left(1+\frac{\tau_1}{\rho}\frac{\partial\rho}{\partial t}\right)\cdot\frac{\partial c}{\partial t}+\tau_1\frac{\partial^2 c}{\partial t^2}=\frac{1}{\rho}\boldsymbol{\nabla}_\mathrm{L}(\rho D\boldsymbol{\nabla}_\mathrm{L}c), \tag{22}$$

where the lower index "L" denotes the Lagrangian representation. Considering the one-dimensional case (the notation $\boldsymbol{\nabla}_\mathrm{L}\to\partial/\partial\varsigma$ will be used, with ς being the relevant new Lagrangian-type space-coordinate) and taking into account the method for describing deformations by Jacobi-determinants $|\boldsymbol{J}|_\mathrm{def}$ also used in Eq. (11), we obtain the the developed form of Eq. (22) as

$$\left(1+\frac{\tau_1}{\rho}\cdot\frac{\partial\rho}{\partial t}\right)\cdot\frac{\partial c}{\partial t}+\tau_1\cdot\frac{\partial^2 c}{\partial t^2} = D(c,T)\cdot\frac{\partial^2 c}{\partial\varsigma^2}+|J|_\mathrm{def}\frac{\partial c}{\partial\varsigma}\cdot\frac{\partial}{\partial\varsigma}\left(\frac{D(c,T)}{|J|_\mathrm{def}}\right). \tag{23}$$

When writing PDE (23), the initial density ρ_0 applied in derivation of Eq. (11) is assumed to be known and be a constant quantity. Moreover, by Eq. (23), we also represent here the correctly developed form of Eq. (22), in contrast to the relevant derivation results published in our own earlier works,[36,37] where some mistakes remained in the expressions relevant to the right-hand side of Eq. (23). In this way, the limit situation emanates directly from the relation (23), as $\tau_1\to 0$ leads to the one-dimensional diffusion equation with state-dependent diffusion coefficient in Lagrangian representation. If $\tau_1\neq 0$, but $\left(1+\frac{\tau_1}{\rho}\cdot\frac{\partial\rho}{\partial t}\right)\to 0$, it will lead to the wave equation. In the second case, we directly obtain a simple one-dimensional wave equation, again with state-dependent diffusion coefficient in Lagrangian representation. It follows also from this wave-equation limit that the density ρ has an exponentially decaying character in time, i.e.,

$$\rho(\varsigma,t)=\kappa(\varsigma)\cdot\mathrm{e}^{-t/\tau_1}, \tag{24}$$

where the still unknown function $\kappa(\varsigma)$ may be determined from the actual boundary conditions. The form (24) for density function is not in contradiction with the wave theory of thermodynamics developed for convection-free cases and predicting constant density,[39] because its exponential decrease versus time may be accompanied by increasing character of the function $\kappa(\varsigma)$. Moreover, it is in agreement with the formula (15) (up to a constant), because by using the definition of the mass fractions $c_k=\rho_k/\rho$, $(1\leq k\leq K)$ for a mixture consisting of K components (i.e., $\rho=\sum\limits_{k=1}^{K}\rho_k$) and for $K=2$, we have $\xi(t)=C_*\cdot\mathrm{e}^{-t/\tau}\leftrightarrow\rho_k=c_k\cdot\rho\propto\kappa(\varsigma)\cdot\mathrm{e}^{-t/\tau_k}$, i.e., there is a full correspondence between Eqs. (15) and (24).

The authors of the monograph[1] state that direct combination of the generalized type constitutive equations (17) with balance equations leads to telegrapher type equation $\tau\frac{\partial^2 c}{\partial t^2}+\frac{\partial c}{\partial t}=D\boldsymbol{\nabla}^2 c$, provided that the quantities τ, ρ and D are of constant values. They use the evolution equations for the mass fractions in the absence of chemical reactions at the beginning of the Chapter 13.1 about extended thermodynamics of diffusion. We think that our result (23) is more general and contains the telegrapher equation in a limit situation as well. Namely, by direct combination of $\rho_0=\rho|\boldsymbol{J}|_\mathrm{def}$ and the first term of the left-hand side from Eq. (23), we obtain

$$\left(1+\frac{\tau_1}{\rho}\cdot\frac{\partial\rho}{\partial t}\right)\cdot\frac{\partial c}{\partial t}\to \left(1-\frac{\tau_1}{|\boldsymbol{J}|_\mathrm{def}}\cdot\frac{\partial}{\partial t}(|\boldsymbol{J}|_\mathrm{def})\right)\cdot\frac{\partial c}{\partial t}, \tag{25}$$

i.e., in the case of large enough values of the Jacobi-determinant $|J|_\mathrm{def}$ which is also supposed not to

change too quickly in time, we directly obtain a telegrapher-type equation. In this case, the right-hand side of Eq. (23) will remain unchanged, i.e., it represents the case of thermodynamically state-dependent diffusion coefficients in the presence of deformations.

6. Development of the general formalism by matrix analysis

In this section, a novel method for direct solutions of PDEs in the case of the coupled transport processes within frame of the formalism initially developed for description of convection-free cases[39] is proposed. This method could also allow a more detailed interpretation of the Curie-principle in connection with multiple eigenvalues of the characteristic equations in the Fourier space. Namely, if we take into account the possibility of existence of the fluxes of different tensorial orders in a given macroscopic dissipative continuum, whose mathematical formalism is well-elaborated within frame of the classical linear irreversible thermodynamics,[38,40] we are in a position to refine this formalism in a remarkable manner. Concretely, from Eq. (8), in the case of convection-free cases ($\boldsymbol{v}=0$), we obtain $\rho\,\dot{a}=\frac{\partial\rho a}{\partial t}$, which, together with the continuity equation, results in $\rho_0\frac{\mathrm{d}a}{\mathrm{d}t}=\rho_0\frac{\partial a}{\partial t}$, where $\rho\to\rho_0=\text{const}$. Then, the differential equation (DE) systems related to coupled transport processes in dissipative systems and characterized by intensive and specific extensive parameters are[39]

$$\begin{aligned}&\frac{\mathrm{d}\boldsymbol{\Gamma}}{\mathrm{d}t}-\hat{\kappa}_0\boldsymbol{\nabla}^2\boldsymbol{\Gamma}=\frac{1}{\rho_0}\hat{s}_0\boldsymbol{\sigma},\quad\left(\hat{\kappa}_0\equiv-\frac{1}{\rho_0}\hat{s}_0\hat{L}_0\right),\\&\frac{\mathrm{d}\boldsymbol{a}}{\mathrm{d}t}-\hat{D}_0\boldsymbol{\nabla}^2\boldsymbol{a}=\frac{1}{\rho_0}\boldsymbol{\sigma},\quad(\hat{D}_0\equiv-\frac{1}{\rho_0}\hat{L}_0\hat{s}_0),\end{aligned}\tag{26}$$

i.e., we arrange these parameters into column vectors, as well as the different contributions of the general entropy production into column vector $\boldsymbol{\sigma}$. In Eq. (26), all the quantities supplemented by index zero denote constant quantities, i.e., this system is a strictly linear one, while the generalized variants of these equations are

$$\begin{aligned}&\frac{\mathrm{d}\boldsymbol{\Gamma}}{\mathrm{d}t}-\hat{\kappa}\boldsymbol{\nabla}^2\boldsymbol{\Gamma}=\frac{1}{\rho}\hat{s}\,\boldsymbol{\sigma},\quad\left(\hat{\kappa}\equiv-\frac{1}{\rho}\hat{s}\hat{L}_0\right),\\&\frac{\mathrm{d}\boldsymbol{a}}{\mathrm{d}t}-(\boldsymbol{\nabla}\cdot\hat{D}\boldsymbol{\nabla})\boldsymbol{a}=\frac{1}{\rho_0}\boldsymbol{\sigma},\quad\left(\hat{D}\equiv-\frac{1}{\rho_0}\hat{L}\hat{s}\right),\end{aligned}\tag{27}$$

with the postulated crucial property that, they are valid for such general systems in which convective motions and various sources of energy, mass etc. are also present.[39] Therefore, we are in a position to study a very general DE system at describing coupled transport processes, but its inhomogeneous character must also be taken into account. Although it is common in the literature on mathematics and mathematical physics, by $\hat{A}$ we do not denote in this section an operator acting in a given, abstract vector-space, but a matrix already represented in it. The precise meaning of $\hat{A}$ will be specialized below, after Fourier-transformation of the system (26). The dimension of the matrices $(\hat{s})_{ij}\equiv\frac{\partial^2 s}{\partial a_i\partial a_j}=s_{ij}$, which are the generalized stiffness moduli obeying Maxwell's symmetry relations $s_{ij}=s_{ji}$, is determined by the number of thermodynamic degrees of freedom ($1\le i,j\le F$). $\boldsymbol{\nabla}^2\equiv\Delta$ is the Laplace-operator, $\hat{L}$ is the conductivity matrix. The basic idea is that in general case, for driving forces of tensorial character, the existence of multiple eigenvalues will also be allowed. The isotropic systems are particularly well-studied from this point of view and the relevant block-diagonal forms of the conductivity matrices obtained by effective applications of the irreducible tensor operators of symmetry groups of the actual macroscopic dissipative continua[38,40] are suitable for foundation of the calculation method we intend to develop here. Firstly, it must be taken into account that the system (26) is characterized by total time derivatives, but the spatial derivatives are of partial character. Due to this fact, it is suitable to apply the Fourier-transformation procedure $f(\boldsymbol{r},t)\to\Im\{f(\boldsymbol{r},t)\}=\tilde{f}(\boldsymbol{k},t)\equiv\int\limits_{\mathbb{R}^3}f(\boldsymbol{r},t)\cdot\mathrm{e}^{-\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}$ on it,where i is the imaginary unit and $k=|\boldsymbol{k}|\in\mathbb{R}$ is a real variable, and we will use the transformed column vectors

$$\begin{aligned}&\boldsymbol{\Gamma}(\boldsymbol{r},t)\to\tilde{\boldsymbol{\Gamma}}(\boldsymbol{k},t),\boldsymbol{a}(\boldsymbol{r},t)\to\tilde{\boldsymbol{a}}(\boldsymbol{k},t),\\&\boldsymbol{\sigma}(\boldsymbol{r},t)\to\tilde{\boldsymbol{\sigma}}(\boldsymbol{k},t).\end{aligned}\tag{28}$$

Secondly, by applying the well-known formula for transformation of derived functions, i.e., by $\Im\left\{\boldsymbol{\nabla}^2 f(\boldsymbol{r},t)\right\}=-k^2\cdot\tilde{f}(\boldsymbol{k},t)$, we obtain the following ODE system:

$$\begin{aligned}&\frac{\mathrm{d}\tilde{\boldsymbol{\Gamma}}(\boldsymbol{k},t)}{dt}+k^2\hat{\kappa}_0\tilde{\boldsymbol{\Gamma}}(\boldsymbol{k},t)=\frac{1}{\rho_0}\hat{s}_0\tilde{\boldsymbol{\sigma}}(\boldsymbol{k},t),\\&\frac{\mathrm{d}\tilde{\boldsymbol{a}}(\boldsymbol{k},t)}{\mathrm{d}t}+k^2\hat{D}_0\tilde{\boldsymbol{a}}(\boldsymbol{k},t)=\frac{1}{\rho_0}\tilde{\boldsymbol{\sigma}}(\boldsymbol{k},t).\end{aligned}\tag{29}$$

The solutions of the systems from Eq. (29) will also be presented for the case of multiple eigenvalues, of their characteristic equations. It can be obtained [48,49] on the basis of detailed applications of Jordan-type block-matrices.[50] Namely, for the general inhomogeneous ODE system $\dot{\boldsymbol{y}}(t)=\hat{A}(t)\,\boldsymbol{y}(t)+\boldsymbol{f}(t)$,with vector-columns $\boldsymbol{y}(t)=(y_1(t),\ldots,y_i(t),\ldots,y_F(t))^{\mathrm{T}}$

composed of functions to be determined, the initial condition $\boldsymbol{y}(t_0) = \boldsymbol{y}_0 = \text{const.}$, and linearization $\hat{A}(t) \to \hat{A} = \text{const}$. Obviously, in our case $\hat{A}$ is of block-diagonal form, whose components can be directly identified with negative values of the matrix-coefficients of the Fourier-transformed column-vectors of intensive and extensive specific thermodynamic quantities in the system (29). If the minimal equation of the matrix $\hat{A}$ has only single roots (s of them), we have the solution of this system in the form of[48,49]

$$\boldsymbol{y}(t;t_0,\boldsymbol{y}_0) = \sum_{p=1}^{s} \mathrm{e}^{\lambda_p(t-t_0)} L_p(\hat{A})\boldsymbol{y}_0 + \sum_{p=1}^{s} \int_{t_0}^{t} \mathrm{e}^{\lambda_p(t-\tau)} L_p(\hat{A}) \cdot \boldsymbol{f}(\tau)\mathrm{d}\tau, \quad (30)$$

where $L_p(\hat{A})$ is a Lagrangian-type interpolation matrix-polynomial. If the minimal equation of $\hat{A}$ also has multiple solutions, the solution of the relevant ODE system will be of the form

$$\boldsymbol{y}(t;t_0) = \sum_{p=1}^{s} \mathrm{e}^{\lambda_p(t-t_0)} \sum_{\upsilon=0}^{\gamma_p-1} (t-t_0)^{\upsilon} H_{p\upsilon}(\hat{A})\boldsymbol{y}_0 + \sum_{p=1}^{s} \int_{t_0}^{t} \mathrm{e}^{\lambda_p(t-\tau)} \times \sum_{\upsilon=0}^{\gamma_p-1} (t-\tau)^{\upsilon} H_{p\upsilon}(\hat{A}) \cdot \boldsymbol{f}(\tau)\,\mathrm{d}\tau, \quad (31)$$

where $H_{p\upsilon}(\hat{A})$ is the Hermitian-type interpolation-(or Lagrange–Sylvester-type-) matrix-polynomial and γ_p is the multiplicity of the root λ_p. Then, in order to derive the complete, applicable solution functions, the inverse Fourier-transformation procedure can be applied in Eqs. (30) and (31).

In order to justify the above-proposed procedure, we also describe here a method, which may illustrate its general validity in solving the general problem of convection-free coupled transport processes discussed in this section. As is known, the potential terms of the form $x^p/p!$ of an independent variable x appear explicitly in the formula of Hermitian polynomials according to the formulae of Faà di Bruno[51] (and discussed in detail in Ref. [52]) as

$$H_n(x) = (-1)^n \sum_{k_1+2k_2=n} \frac{n!\,(-1)^{k_1+k_2}}{k_1!k_2!} \cdot (2x)^{k_1}, \quad (32)$$

allowing connection between Hermitian polynomials as special functions and Hermitian interpolation polynomials, since the latter obey the following relationship:[49]

$$\begin{aligned} \frac{x^p}{p!} &= \sum_{k=1}^{s} \left\{ \frac{x_k^p}{p!} H_{k0}(x) + \frac{x_k^{p-1}}{(p-1)!} H_{k1}(x) \right. \\ &\quad \left. + \cdots + \frac{x_k^{p-q_k}}{(p-q_k)!} H_{kq_k}(x) \right\}, \\ q_k &= \gamma_k - 1, \quad (\gamma_k - 1 \le p); \\ q_k &= p, \quad (\gamma_k - 1 \ge p). \end{aligned} \quad (33)$$

Therefore, the interpolation Hermite-polynomials (more precisely: sum of them) playing a crucial role in the general solution (31) may be expressed as a sum of the usual Hermite-polynomials. This connection between their sums may give us a general method for solution of the systems (26). Namely, we may exploit the property of the Hermitian functions (defined by $\psi_n(x) = \mathrm{e}^{-x^2/2} \cdot H_n(x)$ with $H_n(x)$ being Hermite polynomials of n-th order) with respect to the Fourier-transformation, in the sense of the formula (in the case of the unitary version of the Fourier transformation procedure)

$$\Im\left\{ \mathrm{e}^{-x^2/2} H_n(x) \right\} = (-\mathrm{i})^n \cdot \mathrm{e}^{-k^2/2} H_n(k). \quad (34)$$

The Hermite-functions form an orthonormal basis, which diagonalizes the Fourier transform operator with eigenvalues $(-\mathrm{i})^n$.[53] Its direct application on the abstract vector-components in the solution (31) will result in linear combination of the solutions of (26) we are searching for.

7. Conclusions

Solution of the convection-diffusion PDEs is presented analytically in linear approximation for the case of constant convection velocity flow by use of the advanced symbolic calculation software package MAPLE. This solution is refined stochastically via some very basic scaling relationships of the contemporary percolation theory. It is demonstrated that this simple posteriori coupling of methods of the CIT and percolation theory leads to a good qualitative agreement with results emanating from the earlier nonlinear convection-diffusion theory by Pascal.[19] Then, the balance equations of the non-equilibrium thermodynamics are studied in their most general form and it is shown that deformation as well as the relaxation phenomena can be incorporated into general formalism from the beginning. Both Euler- and Lagrange-representations are used for interconnecting deformation and relaxation processes in two-component systems in a simple, but novel manner. This generalized and more formal new description is in agreement with the earlier ones due to Landau and Lifshitz related to

the secondary viscosity problems. As a direct consequence, the earlier derivation of the telegrapher-type PDE in the case of binary mixtures is presented in a more general form, in comparison with the earlier direct derivation procedures of its. Finally, a novel method is proposed for applying the matrix polynomials to general treatment of coupled transport processes at absence, as well as in the presence of the convection and dissipative source terms.

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