Field-free calculation of heat and mass transfer flows with short-term contact of phases

Renat Sadykov[1], Linar Sabitov[2], Marina Zakirova[2]
[1] Kazan State Power Engineering University, st. Krasnoselskaya, 51, 420066, Kazan, Russia
E-mail: sadykov_r_a@mail.ru
[2] Moscow State University of Civil Engineering, 26 Yaroslavskoe Shosse, 129337, Moscow, Russia
SabitovLS@mgsu.ru, ZakirovaMA@mgsu.ru

Abstract: *Calculation of thermal diffusion and filtration fluxes at the interface by "traditional" methods requires preliminary determination of the potential values (concentration, moisture content, temperature, pressure) in the four-dimensional space of events. Such methods for solving boundary value problems, which provide "extra" information for technical calculations, are usually very laborous and require the use of numerical methods that are not always convenient in engineering practice. The proposed fieldless calculation method allows one to determine on the boundary of the region the gradients from the transfer potentials and, consequently, energy and material flows in the form of a known functional of the potentials at the interface at their short-term contact directly on the matrix of transfer coefficients of the formalized boundary value problem. This method uses the fractional index differentiation operation (fractional differentiation) and is convenient for solving limiting boundary value problems, i.e. when the characteristic size of the contacting phases in the boundary conditions of boundary value problems tends to infinity or the time of their interaction tends to zero.*
KEYWORDS*: DRYING, DYNAMICS, SHORT-TERM CONTACT, PHASE, SURFACE, FOURIER CRITERION, MATHEMATICAL MODELING, HEAT AND MASS TRANSFER, ANALYSIS*

1. Introduction

Calculation of thermal diffusion and filtration flows at the interface by "traditional" methods requires a preliminary determination of the value of the potentials $\overline{P}$ (concentration, moisture content, temperature, pressure) in the four-dimensional space of events $R^4(x_1,x_2, x_3, \tau)=R^4(\bar{x}, \tau)$ [1,2]. Such methods for solving boundary value problems, which provide "extra" information for technical calculations, are very laborious and require the use of numerical methods that are not always convenient in engineering practice [2,3]. The field-free calculation method allows one to determine the gradients from the transfer potentials at the boundary of the region $\left(\vec{\Pi}_{\bar{x}}\big|_{\bar{x}=0}\right)$ at their short-term contact directly on the matrix of transfer coefficients of the formalized boundary value problem. This method uses the fractional index differentiation operation [4].

2. Materials and methods

We present briefly the necessary information about their theory of fractional differentiation.

Definition. For function $\boldsymbol{f(x)}$, given on the segment $[\boldsymbol{a},\ \boldsymbol{b}]$, each of the expressions

$$(D_{a+}^{\alpha} f)(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x \frac{f(t)dt}{(x-t)^a}, \tag{1}$$

$$(D_{b-}^{\alpha} f)(x) = -\frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_x^b \frac{f(t)dt}{(t-x)^a}, \tag{2}$$

is called the fractional derivative or the Riemann-Liouville derivative of order α , 0 < α <1, respectively left-sided right-sided. В (1) and (2) Γ - gamma function, $\boldsymbol{f(x)}$ – piecewise continuous function.

Let us give a sufficient criterion for the existence of fractional derivatives.

Lemma. If a $\boldsymbol{f(x)}$ belongs to the class of absolutely continuous on the segment $[\boldsymbol{a},\ \boldsymbol{b}]$ functions, then $\boldsymbol{f(x)}$ almost everywhere has derivatives $\boldsymbol{D_{a+}^{\ a} f}$ и $\boldsymbol{D_{b-}^{\ a} f}$, $\boldsymbol{0 < \alpha < 1}$, moreover $\boldsymbol{D_{a+}^{\ a} f}$ и $\boldsymbol{D_{b-}^{\ a} f}$ belong to the class measurable on $[\boldsymbol{a},\ \boldsymbol{b}]$ function $\boldsymbol{f(x)}$ *(L_r (a,b), 1≤r< 1/α)*, for whom $\int_a^b |f(x)|^r dx < \infty$ and

$$D_{a+}^{\alpha} f = \frac{1}{\Gamma(1-\alpha)} \left[\frac{f(a)}{(x-a)^a} + \int_a^x \frac{f'(t)dt}{(x-t)^a}\right], \tag{3}$$

$$D_{b-}^{\alpha} f = \frac{1}{\Gamma(1-\alpha)} \left[\frac{f(b)}{(b-x)^a} + \int_x^b \frac{f'(t)dt}{(t-x)^a}\right]. \tag{4}$$

The fractional Liouville derivatives for the semiaxes with the corresponding limits of integration in (1) and (2) are introduced similarly.

3. Theory

Let us consider a mathematical model of interconnected unsteady heat and mass transfer under conditions of short-term contact interaction of phases, which, within the framework of the formalism of linear nonequilibrium thermodynamics based on integral conservation laws, is formulated as a system of linear homogeneous differential equations in the following compact vector-matrix form [5]:

$$\begin{cases} \vec{\Pi}_{j\tau} = K_j \Delta\vec{\Pi}_j,\ x\in\left(0,\ (-1)^j \infty\right),\ \tau\in(\tau_0,\ \tau_k),\ j=1,\ 2 & (5)\\ \vec{\Pi}_j\ (x,\ \tau_0)=\ \vec{\Pi}_j\ (x,\ \tau_k)=\ \vec{\Pi}_j\ \left[(-1)^j\infty,\ \tau\right]=\vec{\Pi}_{j0}\ ,\ \ |x| & (6)\\ k_l\, \vec{\Pi}_{1x}\ (0,\ \tau)=\ k_2\, \vec{\Pi}_{2x}\ (0,\ \tau), & (7) \end{cases}$$

where $\vec{\Pi}_{j}, \vec{\Pi}_{jx}$ – local changes in the vector of transfer potentials $\vec{\Pi}$ dimensions $\boldsymbol{n_j}$ respectively in time $\boldsymbol{\tau}$ and coordinate $\boldsymbol{x}$ in j phase, $\boldsymbol{K = kC^{-l}}$ – constant matrix of system parameters $(n\times n)$, k, C^{-l} – matrices of kinetic coefficients and inverse diagonal matrix of capacitance coefficients, respectively, Δ - component-wise Laplacian, $\boldsymbol{x}$ – coordinate normal to the plane of contact with zero at the interface, $\boldsymbol{\tau_k}$ – duration of contact.

In what follows, omitting the indices of the contacting phases and setting for definiteness $\boldsymbol{x} \in (\boldsymbol{0}, \infty)$, $\boldsymbol{\tau_0 = 0}$ and $\vec{\Pi}(0,\tau)=\vec{\Pi}_s$, we introduce a new vector variable $\vec{\boldsymbol{\theta}} = \vec{\Pi}_{\boldsymbol{0}} - \vec{\Pi}$ (bringing constant initial conditions to zero) and expand the difference between differential operators in time and coordinate in (5) similarly to the difference of squares, then system (5) - (7) will be rewritten as:

$$\begin{cases} (\partial_\tau^{0,5}-\sqrt{K}\partial_x)(\partial_\tau^{0,5}+\sqrt{K}\partial_x)\vec{\theta}=\vec{0}, & (8)\\ \vec{\theta}(x,0)=\vec{\theta}(\infty,\tau)=\vec{\theta}, & (9)\\ \vec{\theta}(0,\tau)=\vec{\theta}_s(\tau). & (10) \end{cases}$$

If the elements of the matrix $k_{ij} > 0$ and det $K > 0$, then the definition of the radical from the matrix is carried out in a continuous unambiguous manner [4]. When the matrix has dimensions 2x2, then the corresponding formulas for determining the radical from the matrix are:

$$b_{11}^2=[k_{11}(k_{11}-k_{22})^2+k_{12}k_{21}(3k_{11}-k_{22})+2k_{12}k_{21}\sqrt{(k_{11}k_{22}-k_{12}k_{21})}]\Delta^{-1},$$

$$\sqrt{K}=\begin{pmatrix} k_{11} & k_{12}\\ k_{21} & k_{22}\end{pmatrix}^{\frac{1}{2}}=\begin{pmatrix} b_{11} & b_{12}\\ b_{21} & b_{22}\end{pmatrix}, \tag{11}$$

where $k_{ij} > 0$, $k_{11}k_{22} > k_{12}k_{21}$,

$$b_{22}^2 = b_{11}^2 - (k_{11} - k_{22})$$

$b_{12}=\frac{k_{12}}{b_{11}+b_{22}}$, $b_{21}=\frac{k_{21}}{b_{11}+b_{22}}$, $b_{11}>0$, $b_{22}>0$, $\Delta=(k_{11}-k_{22})^2+4k_{12}k_{21}$.

In this case, under conditions of linear nonequilibrium thermodynamics, the matrix K, due to the positiveness of the production of entropy, must be positively determined, that is, the following conditions must be satisfied [7-9]:

$$k_{11}>0,\ k_{22}>0,\ (k_{12}+k_{21})^2<4k_{11}k_{22}. \tag{12}$$

Thus, according to the second law of thermodynamics, "eigencoefficients" (or direct coefficients, for example, the coefficients of thermal conductivity, diffusion), k_{ii} must be positive, and the "cross factors" (or drag factors, which are determined by superimposing effects such as thermal diffusion) k_{ij} $(i \neq j)$ can have any sign. Moreover, due to microscopic reversibility [7], the elements k_{ij} must satisfy the Onsager relation, $k_{ij} = k_{ji}$, that is, the matrix is symmetric, and in this case, inequality (12) implies the first inequality in (11) and as a consequence, $b_{12} = b_{21}$. Physically diagonal coefficients k_{ii} determine the intensity of transfer of the i-th flow of a substance (heat, mass of a substance) under the direct action of the thermodynamic force of the same name (for a heat flow, the thermodynamic force will be ∇T −temperature gradient, and for mass flow ∇C – concentration gradient).

Further, considering from physical considerations the equations formed by the right factor of the operator in (8) (the left factor with increasing, for example, the temperature at the interface gives $T_x|_{x=0}>0$, which is physically absurd) and, writing the latter at $x = 0$, we obtain the relation defining $\overrightarrow{\theta_s}$ at the boundary of short-term contact of phases:

$$D^{0,5}\vec{\theta}_s(\tau) + \sqrt{K}\,\vec{\theta}_{sx}(0) = \vec{0}, \qquad (13)$$

For fractional differentiation, the right-hand fractional derivative is used in (13).

The solution of the system of equations (13) with respect to energy and material flows no longer causes difficulties, since the formulas of the fieldless method are applicable to systems of differential equations of parabolic, and for high-intensity processes of heat and mass transfer and hyperbolic types. Calculations of fluxes and a number of heat-mass transfer characteristics for the system of equations (5) with boundary conditions of the first kind and the considered problems of molecular and molecular-molar transfer with mixed boundary conditions of the first and second kind, carried out by the field-free method, are fully confirmed by calculations performed on the fields of transfer potentials proposed in[5].

3. Conclusions

For limiting boundary value problems, the possibility of using a non-field method for calculating heat and diffusion fluxes at interfaces is shown, which essentially uses the operation of a differential fractional index, does not require preliminary determination of fields, allows one to obtain a solution in the form of finite formulas, and is important in applied research.

Analytical solutions of boundary value problems of diffusion and diffusion-filtration heat and mass transfer under mixed boundary conditions of the first and second kind and the calculation of heat and material flows from the obtained temperature and concentration fields are fully confirmed by calculations obtained by the fieldless method.

The results obtained serve the development of the general theory of mathematical modelling, are useful in the formulation of experimental studies on stationary and non-stationary energy and mass transfer, in the analysis and calculation of heat and mass transfer processes in applied research and design.

4. References

[1] Lykov A V and Mikhailov Y A 1963 Theory of heat and mass transfer (Moscow: Gosenergoizdat) vol 536

[2] Tsoi V P 1971 Methods for calculating individual problems of heat and mass transfer (Moscow: Energy) vol 384

[3] Babenko Y I 1986 Heat and Mass Transfer: Method for Calculation of Heat and Diffusion Fluxes (Leningrad: Chemistry) vol 144

[4] Samko S G, Kilbas A A and Marichev O I 1987 Integrals and derivatives of fractional order and some of their applications (Minsk: Science and Technology) vol 688

[5] Gantmakher F A 1967 Matrix Theory (Moscow: The science) vol 576

[6] Prigogine I 2001 Introduction to the thermodynamics of irreversible processes (Izhevsk: Research Center "Regular and Chaotic Dynamics") vol 160

[7] Prigogine I and Kondepudi D 2002 Modern thermodynamics. From heat engines to dissipative structures (Moscow: Mir) vol 461

[8] Eremin V V, Kargov S I, Uspenskaya I A, Kuzmenko N E and Lunin V V 2005 Fundamentals of Physical Chemistry. Theory and Problems (Moscow: Binomial) vol 480

[9] Leontiev A I 2018 Heat and mass transfer theory, 3rd edition

[10] Kartashov E M, Kudinov V A and Kalashnikov V V 2019 Methods for calculating individual problems of heat and mass transfer

[11] Gotovsky M A and Suslov V A 2019 Heat and Mass Transfer

[12] Fedotov A, Baikov V, Pavlyukevich N and Shnip A 2019 Thermophysics: nonequilibrium processes of heat and mass transfer

[13] Burdakov V, Dzyubenko B, Mesnyankin S and Mikhailova T 2019 Thermodynamics (Liters)

[14] Gordeev L, Koltsova E, Vertegel A and Tretyakov Yu 2020 Thermodynamics of irreversible processes and nonlinear dynamics

[15] Semenov V N, Vvedensky A V, Zavrazhnov A Y, Kozaderov O A and Naumov A V 2018 Physical and chemical processes in condensed media and napphase boundaries vol 628

[16] Etkin V A 2018 Accounting for irreversibility in the laws of classical mechanics

[17] Starostin I E and Bykov V I 2018 Analysis and modeling in lumped parameters of dynamics of real physicochemical processes by methods of modern nonequilibrium thermodynamics using system analysis vol 214

[18] Bugrimov A L, Kuznetsov V and Bobrova I A 2018 On the applicability of fractional derivatives in physical models

[19] Beybalaev V D and Shabanova M R 2017 A numerical method for solving a boundary value problem for a two-dimensional heat equation with fractional derivatives vol 244-251