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GENERALIZED VARIATIONAL PRINCIPLE OF MOLAR-MOLECULAR HEAT- AND MASS-TRANSFER PHENOMENA

YU. T. GLAZUNOV
Institute for Advanced Training of Managers and Specialists of Fish Industry,
Kaliningrad Region, U.S.S.R.

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Abstract — Consideration is given to the method of solution of the molar-molecular heat- and mass-transfer problems which is based: on the transformation of the first and the second boundary-value problems for a system of equations into the three boundary-value problems for the heat-conduction equation; on the use of the generalized variational principle written down for the transformed equations; and on the use of the concept of a "layer" for the combined potential of transfer.

NOMENCLATURE

X,	dimensionless spatial coordinate;
Fo,	Fourier number;
ε,	phase transformation criterion;
Pn,	Posnov number;
Ko,	Kossovich number;
Lu,	Luikov number;
Bu,	Bulyguin number;
Lu_p,	criterion for coupling between the molar heat and mass transfer;
Ki_q,	heat-transfer Kirpichyov number;
Ki_m,	mass-transfer Kirpichyov number;
$\theta_1(X, Fo)$,	dimensionless temperature;
$\theta_2(X, Fo)$,	dimensionless potential for mass transfer;
$\theta_3(X, Fo)$,	dimensionless potential for flow mass transfer;
Γ,	shape factor ($\Gamma = 0$ for an infinite plate, $\Gamma = 1$ for an infinite cylinder, $\Gamma = 2$ for a sphere).

INTRODUCTION

FOR THE purpose of intensifying heat- and mass-transfer processes, use is made of high temperatures and pressures. This leads to a pressure gradient inside the moist material which results in molar transfer of the substance. The molecular processes and the molar transfer occurring simultaneously cause a qualitative change in the mechanism of interrelated heat- and mass-transfer. An analytical study of the problem is based on the use of a system of differential equations of the form

$$\frac{\partial\theta_1}{\partial Fo} = \frac{\partial^2\theta_1}{\partial X^2} + \frac{\Gamma}{X} - \frac{\partial\theta_1}{\partial X} - \varepsilon Ko\frac{\partial\theta_2}{\partial Fo} + A_1(X, Fo),$$

$$\frac{\partial\theta_2}{\partial Fo} = Lu\left[\frac{\partial^2\theta_2}{\partial X^2} + \frac{\Gamma}{X}\frac{\partial\theta_2}{\partial X}\right] - LuPn\left[\frac{\partial^2\theta_1}{\partial X^2} + \frac{\Gamma}{X}\frac{\partial\theta_1}{\partial X}\right]$$
$$- Lu_p\frac{Bu}{Ko}\left[\frac{\partial^2\theta_3}{\partial X^2} \quad \frac{\Gamma}{X} + \frac{\partial\theta_3}{\partial X}\right] + A_2(X, Fo),$$

$$\frac{\partial\theta_3}{\partial Fo} = Lu_p\left[\frac{\partial^2\theta_3}{\partial X^2} + \frac{\Gamma}{X}\frac{\partial\theta_3}{\partial X}\right] - \varepsilon\frac{Ko}{Bu}\frac{\partial\theta_2}{\partial Fo} + A_3(X, Fo). \tag{1}$$

Here A_i $(i = 1, 2, 3)$ are the functions accounting for the heat and mass sources and sinks. System (1) may be considered subject to the initial conditions

$$\theta_1(X, 0) = \theta_2(X, 0) = \theta_3(X, 0) = 0; \tag{2}$$

symmetry conditions

$$\frac{\partial\theta_1}{\partial X}(0, Fo) = \frac{\partial\theta_2}{\partial X}(0, Fo) = \frac{\partial\theta_3}{\partial X}(0, Fo) = 0 \tag{3}$$

and the boundary conditions of the first kind

$$\begin{aligned} \theta_1(1, Fo) &= R_1(Fo), \\ \theta_2(1, Fo) &= R_2(Fo), \\ \theta_3(1, Fo) &= R_3(Fo), \end{aligned} \tag{4}$$

or the boundary conditions of the second kind

$$\frac{\partial\theta_1(1, Fo)}{\partial X} - Ki_q(Fo) + NKi_m(Fo) = 0,$$

$$-\frac{\partial\theta_2(1, Fo)}{\partial X} + Pn\frac{\partial\theta_1(1, Fo)}{\partial X} + Ki_m(Fo)$$
$$+ \frac{Bu}{Ko}\frac{Lu_p}{Lu}\frac{\partial\theta_3(1, Fo)}{\partial X} = 0$$

$$\frac{\partial\theta_3(1, Fo)}{\partial X} = B(Fo). \tag{5}$$

Here R_i $(i = 1, 2, 3)$, Ki_m, Ki_q and B are the known functions of time and $N = (1 - \varepsilon)KoLu$.

The available rigorous methods for the study of problems (1)–(5) lead to cumbersome solutions [1], the use of which in practice is found to be difficult in a number of cases.

Let us consider the possibility of obtaining simple approximate variational solutions of the system of molar-molecular heat- and mass-transfer equations (1) under the boundary conditions (2)–(5).

GENERALIZED VARIATIONAL PRINCIPLE

It is known [2] that for the approximate solutions to be obtained, the system of equations (1) may be written in an equivalent form of the system of three non-connected parabolic-type equations with respect to combined potentials

$$Z_i(X, Fo) = p_i\theta_1(X, Fo) + q_i\theta_2(X, Fo) + r_3\theta_3(X, Fo). \tag{6}$$

Let us assume that here and henceforth the subscript i will have the values 1, 2, 3.

The constant coefficients on the RHS of (6) are of the form

$$p_1 = 1,\ q_1 = \frac{v_1^2 - 1}{Pn},\ r_1 = \frac{Lu_p Bu Pn}{(v_1^2 Lu_p - 1)\, LuKo(v_1^2 - 1)}$$

$$p_2 = \frac{Pn}{v_2^2 - 1},\ q_2 = 1,\ r_2 = \frac{Lu_p Bu}{(v_2^2 Lu_p - 1)\, LuKo},$$

$$p_3 = \frac{PnLu_p Bu}{(v_3^2 - 1)(v_3^2 Lu_p - 1)\, LuKo},$$

$$q_3 = \frac{(v_3^2 Lu_p - 1)\, LuKo}{Lu_p Bu},\ r_3 = 1.$$

Here v_i are the roots of the equation

$$v^6 - \beta_1 v^4 + \beta_2 v^2 - \beta_3 = 0,$$

where

$$\beta_1 = 1 + \varepsilon KoPn + \frac{1 - \varepsilon}{Lu} + \frac{1}{Lu_p};$$

$$\beta_2 = \frac{1 - \varepsilon}{Lu} + \left(1 + \varepsilon KoPn + \frac{1}{Lu}\right)\frac{1}{Lu_p};$$

$$\beta_3 = \frac{1}{LuLu_p}.$$

Reference [1] gives the table of the values of v_i for different similarity numbers.

Substitution of (6) transforms the system of equations (1) into three non-connected equations of the heat-conduction type

$$\frac{\partial Z_i}{\partial Fo} = K_i\left(\frac{\partial^2 Z_i}{\partial X^2} + \frac{\Gamma}{X}\frac{\partial Z_i}{\partial X}\right) + M_i(X, Fo), \tag{7}$$

where

$$K_i = \frac{1}{v_i^2};$$

$$M_i = K_i\left[p_i A_1 + q_i\left(PnA_1 + \frac{A_2}{Lu} + \frac{A_3 Bu}{LuKo}\right) + r_1\frac{A_3}{Lu_p}\right]$$

Initial (2) and symmetry conditions (3), respectively, acquire the form

$$Z_i(X, 0) = 0,\quad \frac{\partial Z_i}{\partial X}(0, Fo) = 0, \tag{8}$$

while the boundary conditions of the first and the second kind, (4) and (5), are written down in the form of (9) and (10), respectively [3]:

$$Z_i(1, Fo) = \Phi_i(Fo), \tag{9}$$

$$\frac{\partial Z_i}{\partial X}(1, Fo) = F_i(Fo), \tag{10}$$

where

$$\Phi_i(Fo) = p_i R_1(Fo) + q_i R_2(Fo) + r_i R_3(Fo);$$

$$F_i(Fo) = f_i Ki_q(Fo) + \varphi_i Ki_m(Fo) + \Psi_i B(Fo);$$

$$f_i = p_i + q_i Pn;$$

$$\varphi_i = q_i - (p_i + q_i Pn)N;$$

$$\Psi_i = r_i + q_i\frac{BuLu_p}{KoLu}.$$

With the solutions, Z_i, of equations (7) known, the potentials θ_i sought are expressed in terms of these solutions as:

$$\theta_1 = \frac{\Delta_{\theta_1}}{\Delta},\quad \theta_2 = \frac{\Delta_{\theta_2}}{\Delta},\quad \theta_3 = \frac{\Delta_{\theta_3}}{\Delta}, \tag{11}$$

$$\Delta = \begin{vmatrix} 1 & q_1 & r_1 \\ p_2 & 1 & r_2 \\ p_3 & q_3 & 1 \end{vmatrix} \neq 0;\quad \Delta_{\theta_1} = \begin{vmatrix} Z_1 & q_1 & r_1 \\ Z_2 & 1 & r_2 \\ Z_3 & q_3 & 1 \end{vmatrix};$$

$$\Delta_{\theta_2} = \begin{vmatrix} 1 & Z_1 & r_1 \\ p_2 & Z_2 & r_2 \\ p_3 & Z_3 & 1 \end{vmatrix};\quad \Delta_{\theta_3} = \begin{vmatrix} 1 & q_1 & Z_1 \\ p_2 & 1 & Z_2 \\ p_3 & q_3 & Z_3 \end{vmatrix}.$$

Just as it was done by Biot [4], but ignoring the physical concept behind the quantities used in [4], let us write, for (7), three variational principles of the form

$$\delta V_i + \int_0^1 \left(\frac{1}{K_i}\dot{H}_i + \int_0^X \frac{\Gamma}{X}\frac{\partial Z_i}{\partial X}\mathrm{d}X)\delta H_i \mathrm{d}X\right.$$
$$= Z_i\delta H_i\big|_{X=0} - Z_i\delta H_i\big|_{X=1}, \tag{12}$$

in which

$$V_i = \frac{1}{2}\int_0^1 Z_i^2\,\mathrm{d}X;\quad \dot{H}_i = \frac{\partial H_i}{\partial Fo}.$$

The quantities Z_i and H_i in (12) are connected by the relations

$$Z_i = -\frac{\partial H_i'}{\partial X},\quad H_i = H_i' + \int_0^X\int_0^{Fo} M_i(X, Fo)\mathrm{d}Fo\,\mathrm{d}X, \tag{13}$$

subject to the conditions

$$\delta Z_i = -\frac{\partial}{\partial X}\delta H_i',\quad \delta H_i = \delta H_i'. \tag{14}$$

With (13) and (14) taken into account, it is possible to show that equations (7) follow from (12).

In fact, since

$$\int_0^1 \frac{\partial Z_i}{\partial X}\delta H_i \mathrm{d}X = Z_i\delta H_i\Big|_0^1 - \int_0^1 Z_i\frac{\partial\delta H_i}{\partial X}\mathrm{d}X,$$

then (12) may be written as

$$\int_0^1 \left(\frac{1}{K_i} \dot{H}_i + \frac{\partial Z_i}{\partial X} + \int_0^X \frac{\Gamma}{X} \frac{\partial Z_i}{\partial X} \mathrm{d}X \right) \delta H_i \mathrm{d}X = 0.$$

Since δH_i are arbitrary variations, we have

$$\frac{1}{K_i} \dot{H}_i + \frac{\partial Z_i}{\partial X} + \int_0^X \frac{\Gamma}{X} \frac{\partial Z_i}{\partial X} \mathrm{d}X = 0.$$

From this, on performing differentiation of the both parts of this equality with respect to X and applying the second of relations (13), we obtain equations (7).

If we assume that

$$H_i' = H_i'(q_1, q_2, \ldots, q_m, X, Fo),$$

where $q_j = q_j(Fo)$ $(j = 1, 2, \ldots, m)$ are generalized coordinates, then the second of relations (14) is satisfied automatically, while expressions (13) lead to a system of Lagrange equations of the form

$$\frac{\partial V_i}{\partial q_j} + \int_0^1 \left(\frac{1}{K_i} \dot{H}_i + \int_0^X \frac{\Gamma}{X} \frac{\partial Z_i}{\partial X} \mathrm{d}X \right) \frac{\partial \dot{H}_i}{\partial \dot{q}_j} \mathrm{d}X = Q_{ij} \tag{15}$$

$$(j = 1, 2, \ldots, m).$$

Here

$$Q_{ij} = Z_i \frac{\partial H_i}{\partial q_j} \bigg|_{X=0} - Z_i \frac{\partial H_i}{\partial q_j} \bigg|_{X=1}.$$

The use of the system of equations (15) allows construction of an approximate method for solving the molar-molecular heat- and mass-transfer problems.

VARIATIONAL APPROACH TO SOLUTION OF THE MOLAR-MOLECULAR HEAT- AND MASS-TRANSFER PROBLEMS

Let us first consider the problem at $M_i(X, Fo) \equiv 0$. Introduce the concept of a "layer" of the combined potential Z_i, with the thickness denoted by $\delta_i = \delta_i(Fo)$. A characteristic feature of this "layer" is that beyond its boundaries the value of the respective potential coincides with its initial value while the phenomena of transport of this potential are absent:

$$Z_i(1 - \delta_i, Fo) = 0, \quad \frac{\partial Z_i}{\partial X}(1 - \delta_i, Fo) = 0. \tag{16}$$

The solution of the problem will be divided into two stages. The first stage will take place at $\delta_i < 1$, while the second will start from that moment of Fo_i when the layer thickness takes on the value $\delta_i(Fo_i) = 1$. At the first stage, for the generalized coordinate we shall take the thickness of the layer $q_i(Fo) = \delta_i$, while at the second stage, the value of the combined potential at $X = 0$: $q_i(Fo) = Z_i(0, Fo)$. Approximation of the potentials Z_i will be carried out by quadratic polynomials with respect to the space coordinate which, at the first stage, satisfy the boundary conditions and conditions (16), while at the second stage, the boundary and symmetry conditions. The practical application of the method will be demonstrated at $\Gamma = 0$. At $\Gamma \neq 0$, the sequence of calculations remains without change.

Under the boundary conditions of the first kind, for example, conditions (9) and (16) are satisfied, at the first stage, by the polynomials

$$Z_i = \frac{\Phi_i}{q_i^2} [X - (1 - q_i)]^2. \tag{17}$$

Relations (13), with account for the fact that $M_i \equiv 0$ and $H_i = 0$ at $X = 1 - q_i$, yield the following expression for H_i

$$H_i = -\frac{\Phi_i}{3q_i^2} [X - (1 - q_i)]^3. \tag{18}$$

Substituting (17) and (18) into (15) and integrating with respect to the spatial coordinate from 0 to $1 - q_i$, we obtain, to determine q_i at the first stage, the ordinary differential equations of the form

$$q_i \dot{q}_i = \frac{147}{26} K_i,$$

whence

$$q_i = \left(\frac{147}{13} K_i Fo \right)^{1/2}, \quad Fo_i = \frac{13}{147 K_i}.$$

Substitution of q_i into (17) and of (17) into (11) yields the solution to the problem of interrelated heat and mass transfer at the first stage.

At the second stage, the symmetry conditions (8) and boundary conditions (9) are satisfied by the polynomials

$$Z_i = q_i(1 - X^2) + \Phi_i X^2. \tag{19}$$

With account for the initial condition $H_i = 0$ at $X = 0$, equations (19) and (13) yield

$$H_i = -q_i \left(X - \frac{X^3}{3} \right) - \Phi_i \frac{X^3}{3},$$

while the Lagrange equations (15) take on the form

$$\dot{q}_i = \frac{42}{17} K_i (\Phi_i - q_i),$$

from which

$$q_i = \frac{42}{17} K_i \exp\left(-\frac{42}{17} K_i (Fo - Fo_i) \right) \times \left[\int_{Fo_i}^{Fo} \Phi_i \exp\left(\frac{42}{17} K_i (Fo - Fo_i) \right) \mathrm{d}Fo \right]. \tag{20}$$

Relations (19), (20) and (11) give an approximate solution to the problem at the second stage.

The proposed method of solving the problem of molar-molecular heat- and mass-transfer may be used in the same form also in the case when in the system of equations (1) $A_i = A_i(Fo)$. The order of the solutions remains without change except for the fact that the first condition of (16) is written down as

$$Z_i(1 - \delta_i, Fo) = S_i(Fo) = \int_0^{Fo} M_i(Fo) \mathrm{d}Fo \tag{21}$$

and is used in this form for the construction of the approximating polynomial at the first stage.

The use, for the solution of the molar-molecular heat- and mass-transfer, of the concept of the combined potential "layer" and conjunction with the variational principle, generalized for the purpose, allows an indirect estimation of the accuracy of approximate solutions for the potentials θ_i sought by means of comparing the solutions to the heat-conduction equations for the potentials Z_i, obtained by the variational method, with exact solutions of the corresponding problems.

Expressions (11) governing the transition from the solutions for combined potentials to the solutions for the potentials θ_i sought, may be written in the form

$$\theta_i(X, Fo) = \sum_{j=1}^{3} D_{ij} Z_j(X, Fo). \qquad (22)$$

Here D_{ij} are some constants determined from (11) and expressed in terms of the similarity criteria. If ΔZ_i is an absolute error of the approximate solutions for the combined potentials, obtained by the variational approach, and $\Delta\theta_i$ is an absolute error of the final solutions for the potentials θ_i, then by virtue of (22) we have

$$\Delta\theta_i = \sum_{j=1}^{3} D_{ij} \Delta Z_j.$$

This expression shows that the accuracy of the final solutions depends on the value of the similarity numbers entering into (1) and on the accuracy attained in the solution of equations (7) transformed by the variational approach. In addition, this expression allows an *a posteriori* estimation of errors when there are accurate solutions of the heat-conduction problems for any values of the number Fo and the coordinate X.

A comparison between the variational solutions of (17) and (19) and the exact solutions of equations (7) for constant boundary conditions is presented in Fig. 1. A good agreement of these solutions is observed in a wide range of the Fo number.

CONCLUSION

Application, for the solution of the molar-molecular heat- and mass-transfer problems, of the method based on a simultaneous use of the system of equations transformed to three non-connected equations of the heat-conduction type, of the generalized variational principle written down for the transformed equations, and of the concept of the combined transport potential "layer" makes it possible to obtain simple approximate solutions to these problems. The availability of exact solutions of the heat-conduction problems and of an elementary procedure for the *a posteriori* estimation of errors for them make the variational solutions of the molar-molecular heat- and mass-transfer problems suitable for engineering applications and the method suggested, adequate for engineering calculations.

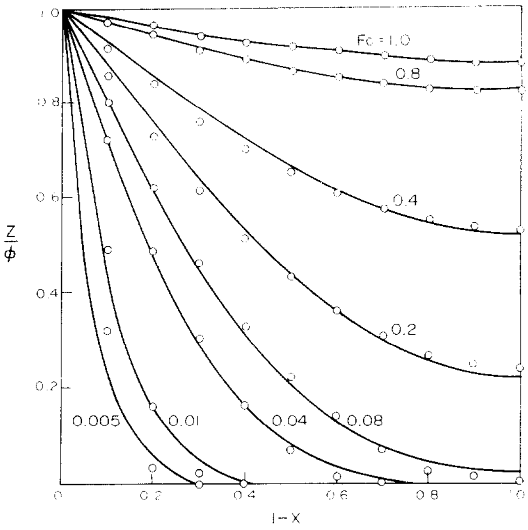

FIG. 1. Comparison between the approximate (circles) and exact solutions (solid lines) for the transformed problem at constant boundary conditions of the first kind for an infinite plate.

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PRINCIPE VARIATIONNEL GENERALISE DES PHENOMENES DE TRANSFERT DE CHALEUR ET DE MASSE

Résumé — On considère la méthode de résolution des problèmes de transfert de chaleur et de masse, basée : (1) sur la transformation des problèmes avec un système d'équations et des conditions aux limites de première et de deuxième espèce en des problèmes avec condition aux limites de troisième espèce ; (2) sur l'application aux équations transformées du principe variationnel généralisé ; (3) sur le concept d'une "couche" pour le potentiel de transfert combiné.

EIN VERALLGEMEINERTES VARIATIONSPRINZIP FÜR MOLEKULARE WÄRME- UND STOFFÜBERTRAGUNGSVORGÄNGE

Zusammenfassung—Es wird eine Lösungsmethode des molekularen Wärme- und Stoffübertragungsproblems behandelt, die auf folgenden Grundzügen beruht: Transformation der ersten und zweiten Randwertaufgabe für ein System von Gleichungen in die drei Randwertaufgaben der Wärmeleitungsgleichung; Anwendung des verallgemeinerten Variationsprinzips auf die Formulierung der transformierten Gleichungen; Verwendung des Konzepts einer 'Schicht' für das kombinierte Potential des Transports.

ОБОБЩЕННЫЙ ВАРИАЦИОННЫЙ ПРИНЦИП ЯВЛЕНИЙ МОЛЯРНО-МОЛЕКУЛЯРНОГО ТЕПЛО- И МАССОПЕРЕНОСА

Аннотация — Рассматривается метод решения задач молярно-молекулярного тепло- и массопереноса, основанный на преобразовании, приводящем первую и вторую краевые задачи для системы уравнений к трем краевым задачам для уравнения теплопроводности; на использовании обобщенного вариационного принципа, записанного для преобразованных уравнений и понятия «слоя» комбинированного потенциала переноса.