ITERATIVE APPROACH TO SOLVING BOUNDARY-VALUE PROBLEMS OF HEAT AND MASS TRANSFER IN REACTIVE MEDIA

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One possible approach is considered to simplifying the procedure of solving heat and mass transfer problems in reacting media.

Heat and mass exchange processes in chemically reactive media are often described by quite complicated systems of differential equations, whose computer solution is associated with certain difficulties. At the same time, for many boundary-value problem of heat and mass transfer in a semi-infinite planar layer of a moving chemically reactive medium, in which the energy conservation equation is written in the form

$$\frac{dT}{dz}\sum_{i=1}^{n} c_i G_i = \frac{d}{dz}\left(\lambda \frac{dT}{dz}\right) + Q, \tag{1}$$

$$\psi_1(T,\ dT/dz) = 0 \text{ for } z = 0, \tag{2}$$

$$\lim_{z\to\infty} T = T_\infty, \tag{3}$$

$$G^* = \sum_{i=1}^{n} G_i = \psi_2(T(0)). \tag{4}$$

Let it be given, besides, that at quite low temperatures, i.e., at temperatures not exceeding some level T_f, the onflow of physicochemical transformations in the medium can be neglected, and let it be assumed that

$$Q = 0, \quad \lambda = \lambda^* = \text{const}, \quad c^* = \left(\sum_{i=1}^{n} c_i G_i\right)/G^* = \text{const}. \tag{5}$$

Following the variable replacement

$$y = z - z_f, \tag{6}$$

where z_j is determined from the condition

$$T(z_f) = T_f, \tag{7}$$

the originally staged problem is transformed to

$$c^* G^* \frac{dT}{dy} = \lambda^* \frac{d^2T}{dy^2}, \quad y \geqslant 0, \tag{8}$$

$$\frac{dT}{dy}\sum_{i=1}^{n} c_i G_i = \frac{d}{dy}\left(\lambda \frac{dT}{dy}\right) + Q, \quad y \in [y_w,\ 0], \quad y_w = -z_f, \tag{9}$$

$$T(0) = T_f, \tag{10}$$

$$\lambda^* \left.\frac{dT}{dy}\right|_{y=+0} = \lambda \left.\frac{dT}{dy}\right|_{y=-0} - \Delta Q_f, \tag{11}$$

$$\psi_1(T,\ dT/dy) = 0 \quad \text{for} \quad y = y_w, \tag{12}$$

$$\lim_{y\to\infty} T = T_\infty, \tag{13}$$

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$$G^* = \psi_2(T(y_w)). \tag{14}$$

In this case it is easily seen that Eq. (8) has an analytic solution, using which one can obtain from relationship (11) the second boundary condition for Eq. (9):

$$\left.\frac{dT}{dy}\right|_{y=-0} = [\Delta Q_f + c^* G^* (T_f - T_\infty)]/\lambda. \tag{15}$$

If the dynamic part of the problem is written in the form

$$\frac{dG_i}{dy} = w_i(T, G_1, \ldots, G_n), \quad i = \overline{1, n}, \tag{16}$$

$$G_i = G^* r_i, \quad i = \overline{1, n}, \quad y = -0, \tag{17}$$

$$\sum_{i=1}^{n} r_i = 1, \tag{18}$$

then the use of relationship (15) for a given value of the total mass velocity of motion of the medium G* makes it possible to reduce the original boundary-value problem to the Cauchy problem (9), (10), (15), (16), (17) with a boundary integration region y_W, whose coordinate must be determined during the integration process of the system of differential equations (9), (16) from the condition of satisfying either equality (12) or equality (14). The unused equality of (12), (14) must close the solution of the problem of determining the total velocity of medium motion G*.

The effectiveness of this approach to solving problem of heat and mass transfer in ractive media is evaluated for the example of solving the problem of quasistationary aerothermal breakdown of glass-plastic materials in a high-temperature gas flow, a problem posed in [1, 2]. In this case T_f is understood to be the pyrolysis temperature of organic bonding, the chemical material composition in the region $[0, y_W]$ is restricted by

$$\mathrm{SiO}_2^{(s)}, \quad \mathrm{C}^{(s)}, \quad \mathrm{SiO}^{(g)}, \quad \mathrm{CO}^{(g)}, \quad \mathrm{H}_2^{(g)}. \tag{19}$$

As a single reaction varying the chemical composition of the material consider a reaction of the type

$$\mathrm{SiO}_2^{(s)} + \mathrm{C}^{(s)} \to \mathrm{SiO}^{(g)} + \mathrm{CO}^{(g)}, \tag{20}$$

while the corresponding flow formation velocities of isolated material components and the intensity of heat separation in it are calculated by the equations

$$\begin{gathered} w_{\mathrm{C}} = -\exp(\beta_R - \alpha_R/T)\, G_{\mathrm{C}} \rho^*/G^*, \\ w_{\mathrm{CO}} = -w_{\mathrm{C}} 28/12, \quad w_{\mathrm{SiO}} = -w_{\mathrm{C}} 44/12, \\ w_{\mathrm{H}_2} = 0, \quad w_{\mathrm{SiO}_2} = w_{\mathrm{C}} 60/12, \quad Q = w_{\mathrm{C}} \Delta Q_R. \end{gathered} \tag{21}$$

The total mass removal rate of silicon dioxide due to the reaction flow (20) is calculated by the equation

$$G_R = \int_0^{y_w} w_{\mathrm{SiO}_2} dy, \tag{22}$$

and to calculate the rate of surface evaporation of this material component we use the Hertz–Knudsen–Langmuir equation

$$G_w = a\varphi \frac{p^*_{\mathrm{SiO}_2} - p_{\mathrm{SiO}_2}}{\sqrt{2\pi R_0 T(y_w)/60}}. \tag{23}$$

The total mass velocity of medium motion G* is uniquely related to the mass breakdown rate of silicon dioxide by a relation of the form

$$\psi_2(T(y_w)) = G^* = -(G_R + G_w)/\varphi. \tag{24}$$

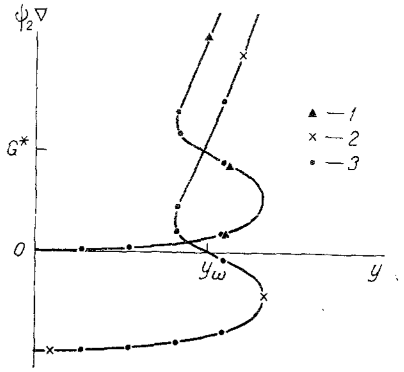

Fig. 1 Typical shapes of the functions $\psi_2(y)$ and $\nabla(y)$: 1) ψ_2; 2 ∇; 3) nodal value of the function (the ordinate axis shows $\psi_2\nabla$; $-G^*$).

As can be easily seen by considering Eq. (23), the calculation of the evaporation rate of silicon dioxide is related to the necessity of determining the chemical composition of the gas mixture over the heated material surface, which is besides also necessary for finding values of the functional dependence $\psi_1(T, dT/dy)$. In this connection it is necessary to point out two facts, intimately related to the calculation difficulties as a whole, the substantial number of gas mixture components over the material surface, and the nonunique dependence of the evaporation rate of silicon dioxide on the temperature of the material surface [1].

The system of nonlinear algebraic equations, describing the boundary conditions on the material surface within the analogy between heat and mass processes and friction in the boundary layer, has a standard form (see, for example, [1, 2]), and the alogrithm of solving the problem considered is practically independent of the shape of the latter. Therefore, it does not seem useful to present here this system of equations.

For a given value of velocity of medium velocity G^* the solution of the problem is sought a follows. Initially, one of the classical numerical methods of solving Cauchy problems for systems of nonlinear ordinary differential equations, solved in the original derivatives by the Runge-Kutta method [3], for example, is seeking a solution of the system of equations (9), (16) in the negatively defined region of the argument y. In this case, in each integration step, along with the unknown functions T, dTdy, and G_i, one also calculates values of the function $\psi_2(T)$ and the sign the mismatch ∇ between $\psi_2(T)$ and G^* (see Fig. 1, where the points on the curves refer to nodal values of the argument y, located at the boundaries of the integration steps).

Besides, during the integration process of this system of equations one controls the generation of situations, when in completing a certain number of integration steps the mismatch sign ∇ changes (from positive to negative in the given case), with subsequent division of the given integration step (by using the trapezoid method, for example) at a certain coordinate y_w, satisfying the condition:

$$\nabla(y_w) = 0. \tag{25}$$

The next element in the problem solution algorithm is determining from the functional dependenced $\psi_1(T, dT/dy)$ th value of the thermal flux g_0, feeding the impenetrable material surface and generating the given value of the mass velocity of the medium velocity G^*.

The ultimate purpose of the calculation is often constructing the dependence $G^*(q_0)$, and in this case the solution of the problem stated is achieved by successive calculations by this algorithm for a given set of values of the parameter G^*. In this case it is important to note the total absence of iterative elements in the problem solution algorithm (only in the regime of purely nonequilibrium evaporation of silicon dioxide, i.e., when $p_{SiO_2} \ll p^*_{SiO_2}$, is the calculation of the chemical composition of the gas mixture over the heated material surface is finding the value of the coordinate y_w sought by the method of successive approximations). These elements are basically generated only by the necessity of searching a specific value of the parameter G^*, corresponding to a given value of the thermal flux q_0. As practice shows, however, the construction of a corresponding iteration process does not usually involve any difficulties, and the number of iterations required does not exceed three to five.

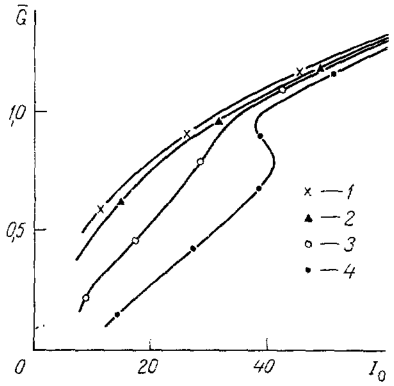

Fig. 2. Dimensionless rate of mass removal of a glass plastic as a function of the drag enthalpy of incoming air flow: 1) $R^* = 0.007$ m; 2) 0.05; 3) 1; 4) 5. I_0, MJ/kg.

Carrying out systematic calculations by the algorithm described above has shown that computer time expenditures are reduced in this case by approximately an order of magnitude in comparison with the case of using traditional iterative methods of solving problems of this kind. At the same time one must keep in mind that a substantial amount of reducing requirements in computer time is basically achieved in the study of substantially nonlinear problems, characterized by a substantial number of iterations required to find the solution sought by traditional successive approximation methods. In studying these relatively simple problems (form the point of view of iterations) the achievement of a substantial effect by using the algorithm discussed above gives rise to problems.

Another restriction on using this algorthm is related to the nonadmissibility of a dependence of the right hand sides of the investigated system of differential equations, written in canonical form, on values of the argument y belonging to the region $[y_w, y_1)$, where y_1 is the current value of the variable of integration. In a number of cases, however, this substantial restriction can be removed to a large extent by replacing the series of functions sought by specially introduced auxiliary functions.

Thus, in particular, in concluding the mechanism of mass removal of glass-plastic materials it remains to consider the melting process of silicon dioxide. As in [2], let the flow of this process in the high-temperature region (i.e., for $T \geq T_f$) be described by an equation of the form

$$\frac{d\Omega}{dy} = -2\rho\varphi\left[\tau_x - p_{xx}(y - y_w)\right]/\mu, \tag{26}$$

while for $T < T_f$

$$\Omega = 0. \tag{27}$$

The total rate of silicon dioxide mass removal in the fluid phase is then written in the form

$$G_L = \int_{y_w}^{0} \Omega dy, \tag{28}$$

while the right hand side of Eqs. (16) for the SiO_2 component and (24) contain additional terms, including the flux of this process:

$$\frac{dG_{SiO_2}}{dy} = w_{SiO_2} - \Omega, \tag{29}$$

$$\psi_2(T(y_w)) = G^* = -(G_R + G_w + G_L)/\varphi. \tag{30}$$

The appearance in the right hand side of Eq. (26) of the parameters y_w and τ_x, whose values can be determined only after completing the integration of the system of equations (9), (16), (26), (29) in the region $[y_w, 0]$, naturally prevents direct use of the algorithm described above for solving the given problem (τ_x depends on the blow-in of material vapor in the boundary layer). If the functions $G_{SiO_2}(y)$ and $\Omega(y)$ are expanded in the auxiliary functions $\eta_j(y)$ and $\xi_k(y)$, i.e., they are represented in the form

$$G_{SiO_2}(y) = \eta_1(y) + y_w\eta_2(y) + \tau_x\eta_3(y), \tag{31}$$

$$\Omega(y) = \xi_1(y) + y_w\xi_2(y) + \tau_x\xi_3(y), \tag{32}$$

and these expansions are then substituted into Eqs. (26), (29), we then obtain a system of equations for determining again the auxiliary functions introduced, containing neither y_w nor τ_x:

$$\frac{d\xi_1}{dy} = 2\rho\varphi p_{xx}y/\mu, \tag{33}$$

$$\frac{d\xi_2}{dy} = -2\rho\varphi p_{xx}/\mu, \tag{34}$$

$$\frac{d\xi_3}{dy} = -2\rho\varphi/\mu, \tag{35}$$

$$\frac{d\eta_1}{dy} = w_{SiO_2} - \xi_1, \tag{36}$$

$$\frac{d\eta_2}{dy} = -\xi_2, \tag{37}$$

$$\frac{d\eta_3}{dy} = -\xi_3. \tag{38}$$

If the solution of this system is carried out with the boundary conditions

$$\xi_1(0) = \xi_2(0) = \xi_3(0) = \eta_2(0) = \eta_3(0) = 0, \quad \eta_1(0) = G^* r_{SiO_2}, \tag{39}$$

it is easily verified that the functions $G_{SiO_2}(y)$ and $\Omega(y)$ thus found satisfy both the original equations (26), (29) and the boundary conditions (17), (27).

If, besides, one neglects the variation of the function $G_{SiO_2}(y)$, related to melting of silicon dioxide, in the energy equation (16), i.e., one replaces in the latter G_{SiO_2} by $G^0{}_{SiO_2}$, determined by an equation of the form

$$G^0_{SiO_2} = \eta_1, \tag{40}$$

which is equivalent to using the well-known Bethe—Adams assumption [4], then, as easily verified, the original boundary-value problem reduces to the Cauchy problem (9), (10), (15)-(17), (33)-(39), but in the functions T, dT/dy, η_1, η_2, η_3, ξ_1, ξ_2, ξ_3, G_C, G_{SiO}, G_{CO}, G_{H_2}.

The errors resulting from the use of assumption (40) usually do not affect substantially the calculation results. Besides, no difficulties occur in constructing an iterative process of refining the solution obtained by replacing Eq. (40) by a relation of the form

$$G^0_{SiO_2}(y) = \eta_1(y) + y^0_w\eta_2(y) + \tau^0_x\eta_3(y), \tag{41}$$

obtained by using in equality (31) the values of the parameters y_w of the previous iteration.

In conclusion we note that the transition from traditional numerical iterative methods of solving problems of heat and mass exchange in reactive media to the solution method discussed in the present study makes it possible to reduce substantially computer time requirements. In particular, the application of this method to solving the problem described in [5] has made it possible to reduce the CPU time by approximately 40 times.

Figure 2 shows, as an example, results of a study carried out by the algorithm of solving heat and mass exchange problems in chemically reactive media as discussed in the present paper, and referring to the scale factor effect on the process of quasistationary aerothermochemical mass removal of a glass-plastic material near the critical point of a blunt body of revolution. The calculations were carried out under the same physicochemical, thermophysical, and kinetic material properties as in [2], while by dimensionless rate of material breakdown we understand the ratio of the parameter G^* to the heat transfer coefficient at the impenetrable surface of the body, selected with the opposite sign.

As seen from the study results presented, on the whole the scale factor has a substantial effect on the process of material mass removal. In this case it is necessary to turn attention to the possibility of occurrence of nonunique dependences of the shape $\bar{G}(I_0)$, not noted in the literature so far. The reason for a dependence of this nature is related to the breakdown in uniqueness of the function $\bar{G}(T(y_w))$, first noted in [5] and related to the appearance on the plot of this portion of the function with an anomalous negative derivative value. With increasing parameter R^* the extension of this anomalous portion of the functional dependence $\bar{G}(T(y_w))$ increases, due to which there also appears the possibility of equilibration of the thermal loads supplied to the surface of the body for various combinations of the basic components of heat exchange, mass removal of the material and radiative heat transfer on its heat surface.

NOTATION

Here z denotes the axis coordinate, related to the surface of the medium and directed toward the internal normal to the latter, n is the number of considered medium components, c_i and G_i are the specific heat capacity of the i-th component of the medium and its mass velocity of motion in the positive direction of the z-axis, λ is the effective heat conduction coefficient of the medium, T is temperature, Q is the source function, characterizing the intensity of heat separation due to flow of physicochemical transformations, ψ_1 and ψ_2 are general nonlinear dependences describing the onflow of heat and mass exchange processes at the surface of the medium, ΔQ_f is the heat separation at the front $T = T_f$, w_i and r_i are the mass rate of formation of the i-th medium component and its weight fraction in the mixture at $y = -0$, α_R, β_R and ΔQ_R are the kinetic reaction constants (20) and its thermal effect, ρ^* is the material density at $T < T_f$, a is the surface accomodation coefficient of the material, $p^*_{SiO_2}$ is the saturated vapor pressure of silicon dioxide, p_{SiO_2} is the partial pressure of silicon dioxide over the material surface, R_0 is the universal gas constant, Ω is the local melting mass rate of silicon dioxide, ρ and μ are the density and dynamic viscosity of the alloy, τ and p are the friction and pressure at the material surface, R^* is the radius of the spherical blunt body, and I_0 is the drag enthalpy of the incoming air flux. Subscripts: x denotes differentiation with respect to the tangential coordinate, and (s) and (g) are the solid phase and gas phase starts of the material.

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