FORMULATION OF COUPLED PROBLEMS OF HEAT AND MASS TRANSFER FOR CHEMICALLY REACTING POLYPHASE MEDIA

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Equations are derived, with the aid of boundary distribution functions, for a description of mass, momentum, and energy balance at the boundary between media in a polyphase stream.

The problem of interaction of polyphase streams with various bodies is quite important, inasmuch as local strains and erosion greatly influence the effectiveness of thermally protective coatings and the flow pattern near bodies in a stream [1, 2]. This problem arises in the formulation of coupled boundary conditions for modeling polyphase streams [3]. Unlike in study [3], in this study will be considered flow of a polydisperse polyphase stream past a body with possible change in the number of particles and in their internal state.

Macrocharacteristics of Interaction. During interaction of particles of condensate phase in the oncoming stream with the surface of a body, there can occur following processes: 1) scattering, i.e., reflection of incident particles by the surface, with or without change in their mass or internal state; 2) erosion, i.e., wear of the body surface by the stream, forming a suspension of the surface material as well as of the condensate phase earlier deposited on the surface; 3) entrapment, i.e., retention of solid or liquid particles in the stream at the interface between the two media, following their penetration depthwise into the body material, their adsorption, etc; 4) secondary wear of body material by the stream as a result of various physicochemical processes in the body bulk as well as at the body surface, also flow of droplets, rollover of particles, etc. All these modes of interaction between the stream and the body material are, naturally, intimately interrelated.

Following the procedure in another study [4], we introduce the functions $H^j_i(\mathbf{u}_i, \mathbf{u}_j, \mathbf{x}_j \to \mathbf{x}_i, t, \tau)$ characterizing the distribution density of streams of scattered particles, $W^j_i(\mathbf{u}_i, \mathbf{u}_j, \mathbf{x}_j \to \mathbf{x}_i, t, \tau)$ characterizing the distribution density of streams of eroded particles, and $I_i(\mathbf{u}_i, \mathbf{x}_i, t)$ characterizing the distribution density of streams of spontaneously emitting particles. Here $\mathbf{x} = \{x_1, x_2, x_3\}$. The thus introduced functions are probability distributions of respective events when a particle with velocity $\mathbf{u}_j$ arrives at point $\mathbf{x}_j$ at an instant of time t and causes emission of particles with velocity $\mathbf{u}_i$ from the point $\mathbf{x}_i$ which a period of time τ.

All these functions have been appropriately normalized [4, 5]. Integrating the distribution densities H^j_i and W^j_i with respect to the velocity of emitted particles yields [5]

$$\sum_i \left[\int (H^j_i + W^j_i)\, d\mathbf{u}_i\right] = 1$$

in the absence of secondary wear. In the general case, however,

$$\sum_j \left[\int (H^j_i + W^j_i)\, d\mathbf{u}_i + S_i\right] = 1.$$

Let us consider an area element with its normal $\mathbf{1}$ (Fig. 1). Since in our case the characteristic length of the particles-and-surface interaction space is smaller than the radius of curvature of the body surface, one can regard the area element as being plane. Within a unit of time the particles impinging on this unit of surface area impart to the latter the following amounts of mass, monentum, and energy:

$$n_j |u_{jl}| m_j;\ n_j |u_{jl}| m_j \mathbf{u}_j;\ n_j |u_{jl}| \left(\frac{1}{2} m_j u_j^2 + E_j + \Pi_j\right) = n_j\, |u_{jl}| H_j^*.$$

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TABLE 1. Characteristics of Interaction during Flow of Two-Phase Stream Past Cone

$(\rho v)_p$, kg/m²·sec	h_p, J/kg	Q_Σ, J/sec	m_Σ, kg/sec	X, N	c_{Dp}	$Q_K S$, J/sec	$Q_T S$, J/sec
0,0798	$2{,}9\cdot10^4$	$2{,}34\cdot10^4$	0,798	11,96	$4{,}90\cdot10^{-5}$	456,89	$2{,}29\cdot10^4$

We now introduce the function

$$M_i^j(\mathbf{u}_i,\ \mathbf{u}_j,\ x_j\to x_i,\ t,\ \tau)=H_i^j+W_i^j,$$

and express the amounts of mass, momentum, and energy worn off from unit surface area as

$$\Lambda_m^{ij}=\int d\tau\int dx\left\{n_j\,|u_{jl}|\int\limits_{u_l>0}M_i^j m_i d\mathbf{u}_i+\int\limits_{u_l>0}I_i m_i d\mathbf{u}_i\right\},$$

$$\Lambda_p^{ij}=\int d\tau\int dx\left\{n_j\,|u_{jl}|\int\limits_{u_l>0}M_i^j m_i\mathbf{u}_i d\mathbf{u}_i+\int\limits_{u_l>0}I_i m_i\mathbf{u}_i d\mathbf{u}_i\right\},$$

$$\Lambda_h^{ij}=\int d\tau\int dx\left\{n_j\,|u_{jl}|\int\limits_{u_l>0}M_i^j\left(\frac{m_i u_i^2}{2}+E_i+\Pi_i\right)d\mathbf{u}_i\right.$$

$$\left.+\int\limits_{u_l>0}I_i\left(\frac{m_i u_i^2}{2}+E_i+\Pi_i\right)d\mathbf{u}_i\right\}.$$

Then the amounts of mass, momentum, and energy received by that unit surface area during its interaction with particles of the j-th fraction and removal from it of particles of the i-th fraction will be

$$L_i^j(\mathbf{u}_j)=n_j\,|u_{jl}|\,m_j-\Lambda_m^{ij};\quad \mathbf{P}_i^j(\mathbf{u}_j)=n_j\,|u_{jl}|\,\mathbf{u}_j-\Lambda_p^{ij};$$

$$Q_i^j(\mathbf{u}_j)=n_j\,|u_{jl}|\,H_j^*-\Lambda_h^{ij}.$$

Now adding the fluxes of all emitted particles will yield the result of action of the j-th fraction on the surface, namely

$$L^j(\mathbf{u}_j)=\sum_i L_i^j(\mathbf{u}_j);\quad \mathbf{P}^j(\mathbf{u}_j)=\sum_i\mathbf{P}_i^j(\mathbf{u}_j);\quad Q^j(\mathbf{u}_j)=\sum_i Q_i^j(\mathbf{u}_j).\tag{1}$$

In order to calulate the total fluxes to the surface, we introduce the distribution function $f_j(\mathbf{u}_j,\ x_j,\ t)$ in the oncoming stream. Multiplying expressions (1) by function $f_j(\mathbf{u}_j,\ x_j,\ t)$ and then integrating with respect to velocities $\mathbf{u}_j$, with $\mathbf{u}_l<0$, yields

$$L^j=\int\limits_{u_l<0}L^j(\mathbf{u}_j)f_j d\mathbf{u}_j;\ \mathbf{P}^j=\int\limits_{u_l<0}\mathbf{P}^j(\mathbf{u}_j)f_j d\mathbf{u}_j;\ Q^j=\int\limits_{u_l<0}Q^j(\mathbf{u}_j)f_j d\mathbf{u}_j.\tag{2}$$

Adding up Eqs. (2) for all fractions of impinging particles yields the total fluxes of mass, momentum, and energy per unit surface area

$$L=\sum_j L^j;\ \mathbf{P}=\sum_j\mathbf{P}^j;\ Q=\sum_j Q^j.\tag{3}$$

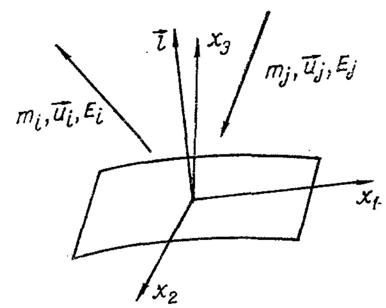

Fig. 1. Schematic diagram of interaction process.

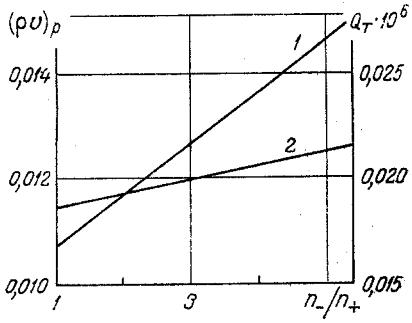

Fig. 2. Dependence of mass flux $(\rho v)_p$, kg/(m²·sec) (curve 1) and of thermal flux Q_T, J/(m²·sec) (curve 2) on interaction multiplicity n_-/n_+ during precipitation of micron spheres on hot substrate in neutral atmosphere.

Assuming that the mixing length for particles at the surface is much smaller than the characteristic lengths of the interaction space and the interaction time is much shorter than the characteristic times, i.e., assuming a Markov process [6], we can represent relations (3) in the form

$$L=\sum_j\sum_i m_j\int\limits_{u_l<0} f_j\left\{n_j|u_{jl}|\left[\delta_{ij}-\frac{m_i}{m_j}\int\limits_{u_l>0} M_i^j d\mathbf{u}_j\right]-\frac{m_i}{m_j}\int\limits_{u_l>0} I_i d\mathbf{u}_i\right\}d\mathbf{u}_j,$$

$$\mathbf{P}=\sum_j\sum_i m_j\int\limits_{u_l<0} f_j\left\{n_j|u_{jl}|\left[\mathbf{u}_j\delta_{ij}-\frac{m_i}{m_j}\int\limits_{u_l>0} M_i^j\mathbf{u}_i d\mathbf{u}_i\right]-\frac{m_i}{m_j}\int\limits_{u_l>0} I_i\mathbf{u}_i d\mathbf{u}_i\right\}d\mathbf{u}_j, \tag{4}$$

$$Q_{\text{к}}=\sum_j\sum_i\int\limits_{u_l<0} f_j\left\{n_j|u_{jl}|\,m_j\frac{u_j^2}{2}-n_j|u_{jl}|\,\frac{m_i}{2}\int\limits_{u_l>0} M_i^j u_i^2\,d\mathbf{u}_i-\frac{m_i}{2}\int\limits_{u_l>0} I_i u_i^2\,d\mathbf{u}_i\right\}d\mathbf{u}_j,$$

$$Q_{\text{т}}=\sum_j\sum_i\int\limits_{u_l<0} f_j\left\{n_j|u_{jl}|\,m_j(E_j+\Pi_j)-n_j|u_{jl}|\,m_j(E_i+\Pi_i)\int\limits_{u_l>0} M_i^j d\mathbf{u}_i-m_i(E_i+\Pi_i)\int\limits_{u_l>0} I_i d\mathbf{u}_i\right\}d\mathbf{u}_j.$$

For convenience, the total energy in the system of equations (4) has been split into kinetic energy Q_K and thermal energy Q_T. In our case the interaction functions are

$$H_i^j(\mathbf{u}_i,\ \mathbf{u}_j,\ t);\ W_i^j(\mathbf{u}_i,\ \mathbf{u}_j,\ t);\ I_i(\mathbf{u}_i,\ t).$$

Coupled Boundary Conditions. The quantities L, $\mathbf{P}$, Q_K, and Q_T will obviously appear as components in the boundary conditions for the coupled problem

$$-\lambda_l\frac{\partial T}{\partial l}=q_w+\varepsilon\sigma_C(T_p^4-T_w^4)+Q_{\text{chem}}+Q_{\text{к}}+Q_{\text{т}}, \tag{5}$$

$$Q_{\text{chem}}=\sum_{\alpha=1}^{N}(R_{\alpha w}q_{\alpha w})_g+\sum_{\beta=1}^{K}(R_{\beta w}q_{\beta w})_p, \tag{6}$$

$$(\rho v)_w=(\rho v)_g+(\rho v)_p;\ (\rho v)_p=L,$$
$$\boldsymbol{\sigma}=\boldsymbol{\sigma}_{\alpha\beta}\mathbf{l}_\beta+\boldsymbol{\tau}_{wg}+\boldsymbol{\tau}_{wp};\ \boldsymbol{\tau}_{wp}=\mathbf{P}. \tag{7}$$

Here Q_{chem} is the energy of chemical transformations at the surface evolving a[illegible] of coupling of N reactions in the carrier medium and K reactions in the incident particles. The stress σ at the boundary between the media consists of the intrinsic stress in the material ($\sigma_{\alpha\beta}l_\beta$-term) and the frictional stress ($\boldsymbol{\tau}_{wg}+\boldsymbol{\tau}_{wp}$). A more precise notation to account for the terms representing the interaction of the carrier medium and the body surface (thermal flux q_w, $(\rho v)_g$, etc.) can be found in an earlier study [7] and is not relevant to the problem under consideration here.

Radiation Model of Interaction. As an example we will consider the case where all distribution functions can be described with the radiation model of interaction

$$H_i^j=\nu_0(d_1,\ d_2,\ \ldots)\,\delta[\mathbf{u}_i-\mathbf{u}_{m0}(u_j^{k0},\ d_1,\ d_2,\ \ldots)],$$
$$W_i^j=\nu_1(b_1,\ b_2,\ \ldots)\,\delta[\mathbf{u}_i-\mathbf{u}_{m1}(u_j^{k1},\ b_1,\ b_2,\ \ldots)],$$
$$I_i=\nu_2(a_1,\ a_2,\ \ldots)\,\delta[\mathbf{u}_i-\mathbf{u}_{m2}(a_1,\ a_2,\ \ldots)].$$

The interaction parameters (a_i, b_i, d_i) can in this case be the surface roughness, the strength characteristics, etc. Functions ν_0, ν_1, ν_2 depend on the impact velocity and the incidence angle as well as on the interaction parameters a_i, b_i, d_i. This model of interaction conforms with reality when the interaction of particles and the carrier medium is weak (treatment of materials, encounter of descending craft with cloud of fairly large particles [1, 8]). Then with a δ-function distribution of particles in the outer stream and with $\Pi_i = \Pi_j = 0$, we have

$$L = \sum_j \sum_i u_{jl}\gamma_{ij};\quad \mathbf{P} = \sum_j \sum_i u_{jl}\mathbf{u}_j\gamma_{ij};\quad Q_{\text{к}} = \sum_j \sum_i u_{jl}\frac{u_j^2}{2}\gamma_{ij}; \tag{8}$$

$$Q_{\text{т}} = \sum_j \sum_i u_{jl}\left(\rho_j E_j - \langle b_{ij}\rangle \rho_i \frac{n_j}{n_i} E_i\right);\ \gamma_{ij} = \rho_j - \langle b_{ij}\rangle \rho_i \frac{n_j}{n_i};$$

$$\langle b_{ij}\rangle = a_j + n_j |u_{jl}| \langle \nu_2(\mathbf{u}_{m2})\rangle;\ a_j = \langle \nu_0 [\mathbf{u}_{m0}(u_j^{k_0})] + \nu_1 [\mathbf{u}_{m1}(u_j^{k_1})]\rangle.$$

Polezhaev's Model [8]. It is evident from Eqs. (8) that, when $E_i \approx E_j = E$, then

$$Q = Q_{\text{к}} + Q_{\text{т}} = (\rho v)_p h_p;\ h_p = \sum_j u_j^2/2 + E.$$

In this case, therefore, h_p can be treated as the effective enthalpy of breakdwon as a result of impact by particles [8]. When the kinetic component of energy is much larger than the thermal component

$$\sum_j u_j^2/2 \gg E,$$

however, then we have the effective breakdown enthalpy according to Polezhaev [8] exactly except for the coefficient.

Busroyd's Model [9]. Assuming that $\rho_i c_{pi} \approx \rho_j c_{pj}$, one can obtain the relation

$$Q_{\text{т}} = \sum_j \sum_i \left[u_{jl}\rho_j c_{pj}\left(T_j - \langle b_{ij}\rangle \frac{n_j}{n_i} T_i\right)\right],$$

identical, except for the coefficient, to the relation [9, 10] for the thermal flux of particles . Within the framework of the radiation model then, the boundary conditions (5) and (6) become

$$-\lambda_l \frac{\partial T}{\partial l} = q_w + \varepsilon\sigma_c (T_p^4 - T_w^4) + \alpha_{\text{к}}\dot{m}_p \frac{u_p^2}{2} + \alpha_{\text{т}}\dot{m}_p (T_p - T_w) + Q_{\text{chem}},$$

$$(\rho v)_w = (\rho v)_g + \alpha_m u_l \rho_p;\ \dot{m}_p = u_l\rho_p, \tag{9}$$

with the form of the accommodation coefficients α_K, α_T, α_m evident from the relations (8).

We will analyze two special cases in the approximation of the radiation model.

1. Flow past Cone. A two-phase stream flows at zero angle of attack past a cone with a vertex half-angle β, assuming that

$$E_i \approx E_j = E_\infty;\ n_j/n_i = 1;\ \nu_2 = 0,$$

and that there is no secondary wear with the number of incident particles equal to the number of emitted ones. We then have

$$(\rho v)_p = u_\infty \gamma \sin\beta;\ P_l = u_\infty^2 \gamma \sin^2\beta;\ \tau_{wp} = u_\infty^2 \gamma \sin\beta\cos\beta;$$

$$Q_{\text{к}} = \frac{u_\infty^3}{2}\gamma\sin\beta;\ Q_{\text{т}} = u_\infty E_\infty \gamma\sin\beta;\ E_\infty = c_{p\infty} T_\infty;\ \gamma = \sum_{j,i}\gamma_{ij}$$

assuming that $\mathbf{u}_j$, $\mathbf{u}_i$, and $\mathbf{l}$ lie in one plane. Assuming further that $\rho_j \approx \rho_i \approx \rho_\infty$, we obtain

$$(\rho v)_p = u_\infty \rho_\infty \varphi(u_\infty^k)\sin\beta;\ P_l = u_\infty^2 \rho_\infty \varphi(u_\infty^k)\sin^2\beta;$$

$$\tau_{wp} = u_\infty^2 \rho_\infty \varphi(u_\infty^k)\sin\beta\cos\beta;\ Q_{\text{к}} = \frac{u_\infty^3}{2}\rho_\infty\varphi(u_\infty^k)\sin\beta; \tag{10}$$

$$Q_{\text{т}} = u_\infty \rho_\infty \varphi(u_\infty^k) E_\infty \sin\beta,$$

where $\varphi(u^k_\infty)$ is the interaction function. A survey of published data indicates that k = 0-6. Under the given assumptions, relations (10) essentially combine the models of brittle and plastic erosion [11]. The total fluxes of mass, monentum, and energy are in this case

$$Q_\Sigma = \int (\rho v)_p h_p dS;\ m_\Sigma = \int (\rho v)_p dS;\ \ X = \int (P_l + \tau_{wp})\, dS.$$

Letting S = const and $\varphi(u^k_\infty) = \varphi_0 + \varphi_1(u^k_\infty - u^k_g) + \ldots$, we obtain the total fluxes, the interaction force, and the drag coefficient c_{Dp} associated with impact on a cone by particles, all given in Table 1 for $\beta = 45°$, $\rho_\infty = 10$, $u_\infty = 107$, $u_g = 110$, $k = 2$, $\varphi_0 = 10^{-4}$, $\varphi_1 = -10^{-8}$, $S = 10$, and $E_\infty = 3 \cdot 10^5$ (all in the International System of units). These values of some of the parameters have been determined experimentally [12] on the assumption that S = const.

2. Flow past Sphere. Inasmuch as $c_{Dp} = 2X(m_p n_p D U^2)^{-1}$ the analogy to flow past a cone under the same assumptions yields

$$c_{Dp} = \text{const}\, u^2_\infty \left[\frac{\varphi_0}{D} + \frac{\varphi_1}{D}(u^k_\infty - u^k_g) + \ldots\right] U^{-2},$$

and from here the relation for the drag coefficient in the Stokes mode of flow

$$c_{Dp} = \frac{24}{\text{Re}}[1 + (\varphi_1/\varphi_0)(u^k_\infty - u^k_g) + \ldots].$$

It is thus evident that, within the framework of the radiation model and under the assumptions made here, the effect of interaction of particles on the interaction coefficient for a sphere is expressed by the second term in the Taylor series expansion of the interaction function $\varphi(u^k_\infty)$.

In the approximation of the radiation model, therefore, one can determine the basic macrocharacteristics of interaction with the aid of two coefficients most readily obtained experimentally.

Model of Equilibrium Precipitation. We now consider the other extreme case, namely that of Maxwell distribution in the outer stream. We assume that the effects of scattering and erosion are negligible, with secondary wear accounted for in the quasiradiation mode. Such an approach is valid for small particles (aerosols) with low concentration and low velocity, those reaching the body surface having moved with direction control (rollover, swinging, migration, etc.) and possible chemical transformations [13]. When

$$f_j = \left(\frac{m_j}{2k\pi T_j}\right)^{3/2} \exp\left(-\frac{m_j u_j^2}{2kT_j}\right),$$

we then have for monodisperse incident and migrating fractions

$$(\rho v)_p = \frac{\rho_+}{4}\left(\sqrt{\frac{2kT_+}{m_+}} - \frac{\rho_- n_+}{\rho_+ n_-}\langle \nu_2 \rangle \pi^{3/2}\right),$$

$$Q_\text{T} = \frac{\rho_+}{4}\left(\sqrt{\frac{2kT_+}{m_+}} E_+ - \frac{\rho_- n_+}{\rho_+ n_-}\langle \nu_2 \rangle \pi^{3/2} E_-\right).$$

Here k is the Boltzmann constant and $0 < \theta_+ \le \pi/2$; $0 \le \theta_- \le \pi$. It is hardly worthwhile to discuss the other terms p and Q_K in this approximation, since they have little effect on the interaction process.

Assuming, along with already known assumptions [14], that the rate of a chemical reaction can be expressed as

$$R_p = k_p \psi(n_+) \exp(-E/(RT_w)),$$

and that the velocity of the carrier medium is very low, also that the medium is chemically neutral, conditions (5) and (6) become

$$-\lambda_l \frac{\partial T}{\partial l} = Q_\text{T} + Q^* k_p \psi(n_+) \exp(-E/(RT_w));\ (\rho v)_w = (\rho v)_p.$$

As an example we will consider precipitation of particles of micron size on a plate during interaction characterized by parameters (in the International System of units) $\rho_+ = 2$, $m_+ = 0.5 \cdot 10^{-16}$, $T_w = 1500$, $Q^* = 55 \cdot 10^2$, $\rho_- = 2$, $c_p = 10^3$, $n_+ = 4 \cdot 10^{16}$, $E/R = 5 \cdot 10^4$, with the assumptions that $T_+ \approx T_-$, $\psi(n_+) = n_+$, and $\nu_2 = \text{const}/n_- = 10^{-19}$. The dependence of $(\rho v)_p$ and Q_T on the interaction multiplicity n_-/n_+ is depicted in Fig. 2.

This demonstrates that the process of heat and mass transfer initiated by particles can, in the approximation of their Maxwell distribution in the outer stream without erosion and scattering, be described with the aid of only one constant which must be determined experimentally.

NOTATION

x_1, x_2, x_3, coordinate axes; u_j, velocity of incident particles; u_i, velocity of emitted particles; t, time; τ, delay time; m_j, mass of particles in the j-th fraction, kine, or type; n, countable number of particles in unit volume; E, internal energy, activation energy; π, potential energy, chemical affinity energy, etc.; f, distribution function in the outer stream; Q_K and Q_T, respectively, kinetic component and the thermal component of energy; λ, thermal conductivity; T, temperature; q, thermal flux; $R_{\alpha g}$, $R_{\alpha g}$, $R_{\beta p}$, $R_{\beta p}$, respectively, rates and the heats of independent heterogeneous chemical reactions between the gas and the immersed surface, between the material of particles and the material of the surface; R, gas constant; Q*, thermal effect; σ, stress; σ_c, Stefan—Boltzmann constant; ε, emissivity; (ρv), mass flux; L, mass flux; P, momentum flux; Q, energy flux; τ_w, frictional stress; k_0 and k_1, coefficients; u_{m0}, u_{m1}, u_{m2}, velocities of dominant emission; a_i, b_i, d_i, interaction parameters; φ, and ν_i, interaction functions; H*, h, enthalpy; c_p specific heat; α, accommodation coefficient; S, surface area; X, force; c_D, drag coefficient; D, characteristic dimension; U, characteristic velocity; Re, Reynolds number; θ, incidence angle; ρ, density; H, W, I, boundary distribution functions; S_i, probability of entrapment. Subscripts: w, surface; p, particle; g, gas; j, precipitating fraction, i, emitted fraction; l, normal component; ∞, outer stream; (+), precipitating fraction; and (—), migrating fraction.

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