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MATHEMATICAL MODELING OF AERODYNAMICS AND PHYSICOCHEMICAL PROCESSES IN THE FREEBOARD ZONE OF A CIRCULATING FLUIDIZED BED FURNACE. 1. STATEMENT OF THE PROBLEM. BASIC AERODYNAMIC EQUATIONS

B. B. Rokhman and A. A. Shraiber

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The authors have obtained a set of equations describing two-dimensional motion of gas and polydisperse char and ash particles in a high-concentration two-phase ascending flow. Interphase interaction, turbulent and pseudoturbulent particle transfer, and effects of the channel walls and mass forces are taken into consideration.

A serious hindrance to power production development is increase of the ash content in the produced fuel and danger of large-scale environmental pollution with emissions of thermal power plants due to high-temperature combustion of powdered fuel in chamber furnaces. With this in view, it is clear that a search for new methods for processing low-grade fuels is urgent. One of these methods is circulating fluidized bed (CFB) combustion. It combines advantages of dust-coal boilers and fluidized bed (FB) furnaces. Since the process occurs at relatively low temperatures, complete burn-out of coke particles is only possible if they stay in the reaction zone for a relatively long time. Therefore, the relations of physicochemical and heat and mass transfer processes in such a system are determined primarily by the aerodynamics and structure of the system. A CFB reactor can be divided into two parts: an FB near the gas distributer and a freeboard zone. The latter, in turn, is divided according to the mode of particle motion into the two zones: the upper (pneumatic transport) zone (PTZ) and the lower (transient) zone (TZ). In the former, ascending material motion takes place at all points of the reactor cross-section, and in the latter, ascending particle motion occurs in the core and descending dense flow of the solid phase takes place in the annular near-wall region. In this article a mathematical model (MM) is suggested for the aerodynamic, heat and mass transfer, and physicochemical processes in the freeboard region of a CFB boiler. In developing an MM it is probably useful to consider separately each of the above mentioned zones. We will start with the aerodynamics of the PTZ, for which the problem is substantially simpler. It should be noted, however, that the model of the flow motion in the PTZ can also be used for the TZ core, which will be considered later.

The discontinous phase will be assumed to consist of n_1 fractions of char and n_2 fractions of ash spherical particles. We will use Euler's description (in the laboratory coordinate system we will consider the point to which particles and gas elements come at different times) and a steady-state two-dimensional (axisymmetric) statement of the problem. It should be noted that in [1, 2], which give the one-dimensional model of motion and heat and mass transfer in a CFB, all parameters of the gas and particles are reactor cross-section-averaged. In this case the effect of the interaction with the wall has to be included rather approximately through the change in the averaged parameters, and consideration of turbulent and pseudoturbulent [3] effects is very difficult. Therefore, one-dimensional models cannot give complete information about the evolution of the state of a two-phase system.

Since in the CFB particle collisions are much more frequent than collisions with the walls, it can be assumed that there will not be any preferable directions of particle rotation in the flow*. Therefore, it is possible to omit the

* More exactly, axial velocities of the particles are much larger than transverse ones so that the preferable directions of their angular velocity vector Ω lie in the horizontal plane; however, the distribution of the directions Ω is practically uniform (see also [4])

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equation of the particle moment of momentum transfer, and the averaged Magnus force should be small compared to the other factors. Estimates of the contributions of viscous and concentration migrations [5] show that under the conditions in a CFB the corresponding drift velocity is at least an order smaller than the characteristic transverse fluctuation velocity. Thus, the equations of the averaged particle motion should include interphase interaction (aerodynamic resistance and Safman's forces), particle collisions, and the mass force.

Use will be made of the boundary layer approximation, i.e., $\bar{v} << \bar{u}$ and $\partial/\partial z << \partial/\partial r$ will be assumed. In considering turbulent and pseudoturbulent effects, ordinary assumptions will be made: $u' << \bar{u}$, but $\bar{v}' \sim \bar{v}$ (u' and v' are characteristic fluctuation components). It will also be assumed that in the transverse direction turbulent transfer is comparable with convective transfer and in the longitudinal direction the former is much smaller than the latter. If $\partial\bar{p}/\partial r$ is neglected (this quite reasonable under the conditions considered), the equation for the averaged radial gas velocity can be omitted.

The initial equations can be obtained by applying Reynolds's procedure to the actual equations of mass and momentum conservation for the gas and particles. Since the derivation of these equations is similar to that described in [6], we will present this system in the final form:

$$\frac{\partial}{\partial z}(\bar{\rho}_g \bar{u}_g) + \frac{1}{r}\frac{\partial}{\partial r}[r(\bar{\rho}_g \bar{v}_g + \overline{\rho_g' v_g'})] = 0\,; \tag{1}$$

$$\frac{\partial}{\partial z}(\bar{\beta}_i \bar{u}_i) + \frac{1}{r}\frac{\partial}{\partial r}[r(\bar{\beta}_i \bar{v}_i + \overline{\beta_i' v_i'})] = 0 \tag{2}$$

$$(i = j,\, l;\quad j = 1,\, 2,\, \ldots,\, n_1;\quad l = 1,\, 2,\, \ldots,\, n_2);$$

$$\bar{\rho}_g \bar{u}_g \frac{\partial \bar{u}_g}{\partial z} + (\bar{\rho}_g \bar{v}_g + \overline{\rho_g' v_g'})\frac{\partial \bar{u}_g}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\mu_g \frac{\partial \bar{u}_g}{\partial r} - \bar{\rho}_g \overline{u_g' v_g'}\right)\right] - \frac{\partial \bar{p}}{\partial z} - \sum_i \bar{F}_{iz}\,; \tag{3}$$

$$\rho_i\left[\bar{\beta}_i \bar{u}_i \frac{\partial \bar{u}_i}{\partial z} + (\bar{\beta}_i \bar{v}_i + \overline{\beta_i' v_i'})\frac{\partial \bar{u}_i}{\partial r}\right] = -\frac{\rho_i}{r}\frac{\partial}{\partial r}(r\beta_i \overline{u_i' v_i'}) + \bar{F}_{iz} + \bar{C}_{iz} - \rho_i \bar{\beta}_i g\,; \tag{4}$$

$$\rho_i\left[\bar{\beta}_i \bar{u}_i \frac{\partial \bar{v}_i}{\partial z} + (\bar{\beta}_i \bar{v}_i + \overline{\beta_i' v_i'})\frac{\partial \bar{v}_i}{\partial r}\right] = -\frac{\rho_i}{r}\frac{\partial}{\partial r}[r(\bar{v}_i \overline{\beta_i' v_i'} + \bar{\beta}_i \overline{v_i'^2})] + \bar{F}_{ir} + \bar{C}_{ir} + \rho_i \bar{\beta}_i \overline{w_i'^2}/r\,. \tag{5}$$

Continuity equations (1) and (2) include axial and radial convective and fluctuation mass transfer. In the right-hand side of (3) viscous and turbulent stresses, the pressure gradient, and the inverse particle effect appear. Equations of particle motion (4) and (5) include the Reynolds stresses, gravity forces, collision forces, forces of interaction with the gas, and centrifugal forces induced by transverse velocity fluctuations. It can easily be seen that the term $(\partial/\partial r)(r\beta_i v_i'^2)$ in (5) includes the turbophoresis effect (particle displacement toward decreasing fluctuation rates). Integration of (1) over the reactor cross-sectional area with $\bar{v}_{gw} = 0$, $(\rho_g' v_g')_w = 0$ gives the equation of gas flowrate conservation:

$$G_g = 2\pi\bar{\rho}_g \int_0^R \bar{u}_g\, r dr \tag{6}$$

(naturally, for isothermal conditions $\partial\bar{\rho}_g/\partial r = 0$ follows from $\partial\bar{p}/\partial r = 0$). Using formula (6) one can find gas density from the function $\bar{u}_g(r)$, known for every cross-section z, and the gas pressure is found from the equation of state.

Then, it is necessary to determine the turbulence parameters of gas. To do this, use will be made of the one-parameter model, i.e., system (1)-(6) will be supplemented with the equation of transfer of kinetic energy of turbulent gas fluctuations $k_g = 0.5(u_g'^2 + v_g'^2 + w_g'^2)$:

$$\overline{\rho}_g \overline{u}_g \frac{\partial k_g}{\partial z} + (\overline{\rho}_g \overline{v}_g + \overline{\rho_g' v_g'}) \frac{\partial k_g}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \left[\mu_g \frac{\partial k_g}{\partial r} - 0.5 \overline{\rho}_g \overline{v_g' (u_2'^2 + v_g'^2 + w_g'^2)} \right] \right\} -$$

$$- \overline{\rho}_g \overline{u_g' v_g'} \frac{\partial \overline{u}_g}{\partial r} + \Gamma_p - \overline{\rho}_g (\varepsilon + \varepsilon_p) . \tag{7}$$

In the right-hand side of equation (7) the first term describes molecular and turbulent transfer of the fluctuation energy, the second and third terms describe its generation due to the energy of averaged motion and flow turbulization in the particle wake, and the fourth term describes dissipation due to gas viscosity and the presence of a disperse phase [3, 6]. For calculation of the correlations of the fluctuation parameters of the gas appearing in (1), (3) and (7), we will use the Boussinesq hypothesis and its analogs

$$\overline{\rho_g' v_g'} = - D_t \frac{\partial \overline{\rho}_g}{\partial r} = 0 ; \quad \overline{u_g' v_g'} = - \nu_t \frac{\partial \overline{u}_g}{\partial r} ; \quad \overline{v_g' (u_g'^2 + v_g'^2 + w_g'^2)} = - \frac{\nu_t}{\sigma} \frac{\partial k_g}{\partial r} \tag{8}$$

(here σ is an empirical constant). The value of ν_t in (8) can be determined using the recommendations of [7].

In order to find correlations of the fluctuation parameters of particles ($\overline{v_i'^2}$, $\overline{w'^2}$, $\overline{u_i'}$, v_i', $\overline{\beta_i' v_i'}$, see (2), (4), and (5)), first of all, it is necessary to determine the intensity of their random motion. As is known, large particles ($\delta \sim 10^{-4}$ m and larger), which constitute a substantial part of the discrete flow mass in the CFB, are entrained by turbulent fluctuations of the carrier quite weakly. Fine particles, which are entrained to a great extent likewise cannot be brought into intense fluctuational motion by the turbulent mechanism, since under the conditions considered the kinetic energy k_g of gas fluctuations markedly decreases because of dissipation on particles (the term ε_p in (7)). Nevertheless, when the concentrations in the flow are not very small, particles are involved in random motion induced by the mechanism of particle collisions [3, 8]; in this case pseudoturbulent energy is generated due to the energy of the averaged particle motion, and the potential energy of the gas is transformed into the latter.

Thus, it will be assumed subsequently that the random particle motion (its energy is defined by $k_i = 0.5(\overline{u_i'^2} + \overline{v_i'^2} + \overline{w_i'^2})$) consists of turbulent and pseudoturbulent components. Naturally, k_i cannot be found with the use of the locally homogeneous approximation (in a way similar to that used in [6] for calculation of the intensity of purely turbulent particle motion). In this case it is necessary to take account of generation of the random energy due to the averaged motion, its dissipation, and transfer by different mechanisms. In order words, it is necessary to construct the equation of transfer of the energy of random particle motion, similar to (7). It should be noted that for turbulent flows this equation was used (probably for the first time) in [9]. However, in that study only the terms describing the convective transfer and fluctuation slip are taken into consideration. In [7] more adequate transfer equations are derived for $\overline{v_p'^2}$, $\overline{w_p'^2}$, etc. (also with just turbulent motion taken into account). As regards random particle motion of pseudoturbulent origin, for gas suspensions this question has been studied very inadequately and in the existing models (for example, [5]), this factor is neglected. It seems worthwhile to pay attention to papers [10, 11], devoted to investigation of the particle motion in highly concentrated systems (fluidized or packed beds). In [10] the authors analyze the case of concentrations close to the maximum β_{max}, where displacements of particles have an order of magnitude substantially smaller than their size. They use the ordinary hydrodynamic equation for each of the phases. In these equations the transfer coefficients are calculated from very simple kinetic considerations. In [11] the one-particle f and two-particle $f^{(2)}$ velocity distributions of particles are introduced (f is governed by Boltzmann's equation) and from the equation of transfer of traits a general form of the hydrodynamic equations of conservation of mass, momentum, and energy of random particle motion is obtained. Next, for calculation of the terms in this equation it is assumed that the function f is Maxwellian and $f^{(2)}$ is a product of one-particle functions with the normalization factor $0.6[1 - (\beta/\beta_{max})^{1/3}]^{-1}$ (in this case not quite elastic particles with smooth surfaces are considered). Evidently, formal extension of the gas kinetic relations to the mechanics of multiphase media could not be considered reasonable. It should be also noted that the authors of [10, 11] consider only monodisperse material, neglecting gas turbulence, and the particle roughness is either neglected [11] or analyzed in a special case [10]. In what follows, some of the relations from [10, 11] will be compared with the present results.

In the construction of a model of random particle motion in a gas suspension flow two methods can be used:

a) separate determination of parameters of turbulent and pseudoturbulent motions followed by finding the total energy of random motion;

b) determination of the total energy from one general equation.

It is likely that method (a) results in simpler relations; however, the problem of adequately combining and summing the results is very complicated and requires adoption of particular hypotheses, whose justification is connected with additional difficulties. Therefore, method (b) will be used here. For the derivation of the transfer equation for k_i, it is necessary, first of all, to obtain the equation for fluctuation particle motion; just as in [6, 7] we have

$$\rho_i [\beta_i \mathbf{V}_i \cdot \nabla \mathbf{V}_i' + (\beta_i \overline{\mathbf{V}}_i)' \cdot \nabla \overline{\mathbf{V}}_i] = \mathbf{F}_i' + \overline{\mathbf{C}}_i + \rho_i \mathbf{g} \beta_i' + \nabla \overline{(\beta_i \mathbf{V}_i)' \mathbf{V}_i'} \tag{9}$$

(here β_i and $\mathbf{V}_i$ are actual values of the parameters). Since subsequently the projections in (9) will be multiplied by the fluctuation velocity components and averaged, it is clear that after these manipulations the last term in the right-hand side of (9) will be zero. Two simplifying assumptions will be used: (1) as was shown by estimates, the resistance force exceeds the Safman force over almost the whole cross-sectional area of the channel, so that the latter will be neglected; (2) fluctuations of the gravity force will also be neglected. The fluctuation component of $\mathbf{C}_i$ is related with random position of the impact line rather than with velocity or concentration fluctuations (in particular, $\overline{\mathbf{F}}_i'$) with prescribed velocities of the interacting particles. Therefore, conventional methods of turbulence theory cannot be used for calculation of $\overline{\mathbf{C}_i' \cdot \mathbf{V}_i'}$ (which describes generation and dissipation of the energy of random motion due to collisions). These components of the final equation of transfer will be determined separately from analysis of the dynamics of the collision process. In view of the above, the corresponding terms in (9) will be omitted and the equation will be projected onto the coordinate axes. As an example, we will give the projection onto the r axis

$$\rho_i \beta_i \left(u_i \frac{\partial v_i'}{\partial z} + v_i \frac{\partial v_i'}{\partial r} + \frac{w_i}{r} \frac{\partial v_i'}{\partial \varphi} - \frac{w_i w_i'}{r} \right) +$$

$$+ \rho_i \left[(\beta_i u_i)' \frac{\partial \overline{v}_i}{\partial z} + (\beta_i v_i)' \frac{\partial \overline{v}_i}{\partial r} + (\beta_i w_i)' \frac{\partial \overline{v}_i}{r \partial \varphi} - \frac{1}{r} (\beta_i w_i)' \overline{w}_i \right] = F_{ir}' \tag{10}$$

(here a general case is considered and axial symmetry of the problem is neglected; therefore terms containing $\overline{w_i}$ and $\partial/\partial\varphi$ appear here). Then, equation (10) is multiplied by $\overline{v_i}$ and averaging is performed in the resultant equation. Equations for $u_i'^2$ and $w_i'^2$ can be written in the same way. Summing up the three equations, using axial symmetry of the problem and the boundary layer approximation, and neglecting the concentration fluctuations compared to velocity fluctuations and the other small terms will result in transforming the equations of transfer of energy of random motion of particles i to the form

$$\rho_i \left[\overline{\beta}_i \overline{u}_i \frac{\partial k_i}{\partial z} + (\overline{\beta}_i \overline{v}_i + \overline{\beta_i' v_i'}) \frac{\partial k_i}{\partial r} \right] = \frac{\rho_i}{2r} \frac{\partial}{\partial r} [r \overline{\beta}_i \overline{v_i' (u_i'^2 + v_i'^2 + w_i'^2)}] -$$

$$- \rho_i \overline{\beta}_i \overline{u_i' v_i'} \frac{\partial \overline{u}_i}{\partial r} + \overline{\mathbf{F}_i' \cdot \mathbf{V}_i'} + K_i, \tag{11}$$

where $K_i = K_i^* - K_i^{**}$, K_i^* describe the generation and K_i^{**} describes the dissipation of the pseudoturbulent energy due to collisions. In equation (11) the first term in the right-hand side describes the transfer of k_i by random particle motion, the second term describes the transition of the energy of averaged motion into fluctuation energy, and the third, the generation and dissipation of the fluctuation energy due to the aerodynamic resistance force. As was noted earlier, k_i includes both turbulent and pseudoturbulent energies, and therefore the correlations in (11) (except for $\overline{u_i'v_i'}$) should be calculated with account for both mechanisms. However, the term containing the averaged velocity gradient describes just the turbulent effects since generation of pseudoturbulence due to averaged motion is described by the term K_i^*. Correlations of the parameters of particles are calculated similarly to (8). It should be noted in conclusion that in [11] the equation of transfer of the energy of random motion of monodisperse material has a structure similar to that of (11) but includes only the mechanism of particle collisions.

NOTATION

z, r, φ, longitudinal, radial, and transverse coordinates; p, pressure; ρ, density; β, true volume concentration; V, velocity vector; u, v, w, its projections onto the axes z, r, and φ; ν, μ, kinematic and dynamic viscosities; F_i, force of interphase interaction of the i-th fraction per unit volume of the two-phase mixture; C_i, force of interphase collisions; g, gravitational acceleration; G, mass flowrate; R, reactor radius; k, kinetic energy of fluctuation motion; D, diffusion coefficient. Subscripts: g, gas; i, j, l, number of the particle fraction; w, wall; t, turbulent analog; superscripts: –, ′, averaged and fluctuation components.

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