Journal of Engineering Physics and Thermophysics, Vol. 67, No. 1-2, 1994

MATHEMATICAL MODELING OF THE AERODYNAMICS AND PHYSICOCHEMICAL PROCESSES IN THE FREE BOARD ZONE OF A CIRCULATING FLUIDIZED BED FURNACE.
IV. HEAT AND MASS TRANSFER AND COMBUSTION

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UDC 536.46:662.62:66.096.5

A mathematical model describing the motion of a highly concentrated coke-ash mixture in the pneumatic transport region within the free board zone of a circulating fluidized bed reactor was developed earlier in [1–3]. In the present work it is extended to the case of a nonisothermal flow with heterogeneous combustion of carbon. Equations of mass, momentum, and energy conservation are obtained for the gas components and the coke fractions. Distinctive features of the heat transfer, combustion, and particle motion are investigated numerically.

In the previous parts of the present work [1–3] a system of equations was obtained for axisymmetric motion of gas and polydisperse coke and ash particles in the pneumatic transport region within the free board zone (FBZ) of a circulating fluidized bed reactor, and some numerical results were presented. The system includes equations of transfer of mass, momentum, and kinetic energy of fluctuation motion of gas and particles (see [1], Eqs. (1)-(5), (7), and (11)). In what follows, these results will be extended to the case of a nonisothermal flow with combustion of the particles.

As was done in [4], it will be assumed that volatiles have enough time to evolve from the coal particles in the fluidized bed section, and in the FBZ heterogeneous reactions of carbon with reactant gases occur on the outer surface of impermeable spherical particles. In this case the reaction rates observed are determined from the model of a "compressible" nonreacting core. When anthracite burns in air, it is sufficient to consider the interaction of coke particles with oxygen and carbon dioxide in the stoichiometric scheme of the reactions:

$$C + O_2 = CO_2 + Q_1\,; \quad C + 0.5O_2 = CO + Q_2\,; \quad C + CO_2 = 2CO - Q_3\,. \tag{1}$$

In accordance with Eq. (1), the gas will be assumed to consist of four components, i.e.,

$$\rho_g = \sum_{m=1}^{4} C_m M_m\,, \tag{2}$$

where the subscripts $m = 1-4$ refer to O_2, CO_2, CO, and N_2.

All hypotheses and simplifying assumptions enumerated in [1] (in particular, the boundary layer approximation) will be used here. As before, the pressure of the gas will be assumed constant in a cross section of the flow, but unlike [1], the density of the gas will change in accordance with changes in the temperature. Just as in [1], the equations of evolution of the state of the system can be obtained by applying Reynolds's procedure to the actual equations of mass, momentum, and energy conservation for the phases (the derivation is similar to that of [5] and to save space it is omitted here).

The continuity equations of the m-th component of the gas have the form

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Institute of Problems of Energy Conservation, Academy of Sciences of Ukraine, Kiev, Ukraine. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 67, Nos. 1-2, pp. 32-38, July-August, 1994. Original article submitted June 16, 1992.

$$\frac{\partial}{\partial z}(\overline{C}_m\overline{u}_g)+\frac{1}{r}\frac{\partial}{\partial r}[r(\overline{C}_m\overline{v}_g+\overline{C'_m v'_g})]=6\sum_j(\overline{C}^s_{mj}-\overline{C}_m)\frac{\overline{\beta}_j\overline{\alpha}_{mj}}{\delta_j}, \tag{3}$$

where $\sum_j$ means the sum over the fractions of the coke particles (as in [1], the subscripts j and l refer to coke and ash particles, respectively, and $\sum_i$ denotes the sum over all coke and ash fractions). Averaged concentrations of gas components on the particle surface $\overline{C}^s_{mj}$ are determined from the balance relations for oxygen, carbon dioxide, and carbon monoxide flows:

$$-\overline{\alpha}_{1j}(\overline{C}^s_{1j}-\overline{C}_1)=(\overline{K}_{1j}+\overline{K}_{2j})\overline{C}^s_{1j};$$

$$\overline{\alpha}_{2j}(\overline{C}^s_{2j}-\overline{C}_2)=\overline{K}_{1j}\overline{C}^s_{1j}-\overline{K}_{3j}\overline{C}^s_{2j};$$

$$\overline{\alpha}_{3j}(\overline{C}^s_{3j}-\overline{C}_3)=2(\overline{K}_{2j}\overline{C}^s_{1j}+\overline{K}_{3j}\overline{C}^s_{2j}).$$

Summation of Eqs. (3), multiplied by M_m, over m gives the continuity equation for the gas

$$\frac{\partial}{\partial z}(\overline{\rho}_g\overline{u}_g)+\frac{1}{r}\frac{\partial}{\partial r}[r(\overline{\rho}_g\overline{v}_g+\overline{\rho'_g v'_g})]=6\sum_j(\overline{\rho}^s_{gj}\overline{\alpha}^s_j-\overline{\rho}_g\overline{\alpha}_j)\frac{\overline{\beta}_j}{\delta_j}, \tag{4}$$

where

$$\overline{\alpha}^s_j=\sum_m\overline{C}^s_{mj}M_m\overline{\alpha}_{mj}\Big/\left(\sum_m\overline{C}^s_{mj}M_m\right);\quad \overline{\alpha}_j=\sum_m\overline{C}_mM_m\overline{\alpha}_{mj}\Big/\left(\sum_m\overline{C}_mM_m\right)$$

($\overline{\rho}^s_{gj}$ is calculated similarly to Eq. (2)).

For the reacting coke particles two continuity equations are written (it is taken into consideration that the calculated concentration does not change due to combustion):

$$\frac{\partial}{\partial z}(\overline{\beta}_j\overline{u}_j)+\frac{1}{r}\frac{\partial}{\partial r}[r(\overline{\beta}_j\overline{v}_j+\overline{\beta'_j v'_j})]=-6[\overline{\alpha}_{2j}(\overline{C}^s_{2j}-\overline{C}_2)+\overline{\alpha}_{3j}(\overline{C}^s_{3j}-\overline{C}_3)]M_C\overline{\beta}_j/(\delta_j\rho_j); \tag{5}$$

$$\frac{\partial}{\partial z}(\overline{n}_j\overline{u}_j)+\frac{1}{r}\frac{\partial}{\partial r}[r(\overline{n}_j\overline{v}_j+\overline{n'_j v'_j})]=0 \tag{6}$$

(M_C is the molecular weight of carbon). At each point of the flow the size of the coke particles is easily found from the known $\overline{\beta}_j$ and $\overline{n}_j$ ($\delta_j=(6\overline{\beta}_j/\pi\overline{n}_j)^{1/3}$). Equations (4) and (5) differ from similar equations (1) and (2) in [1], obtained for a nonreacting flow, in the right-hand side, which, like that in Eq. (3), includes the effect of heterogeneous reactions (1). It should be noted that in the right-hand side of (3)-(5) and in the subsequent equations, corrrelations containing fluctuations of the concentrations of the components and the diffusion mass transfer are omitted since their contributions must be comparatively small for rather large particles (see [5]) and the calculation is very difficult. Naturally, for the ash particles the continuity equation preserves the form of Eq. (2) of [1].

Let the substance transferred from the j-th coke fraction to the gas phase as a result of reactions (1) leave behind its fraction with the parameters of the particles ($\overline{u}_j$, $\overline{v}_j$, $\overline{k}_j$, $\overline{h}_j$). Then, the equations of axial (4) and radial (5) motion of the particles presented in [1] and Eq. (11) concerning the kinetic energy of random motion of the particles presented in [1] remain in force in the case considered. The equation of axial motion of the gas has the form

$$\overline{\rho}_g\overline{u}_g\frac{\partial\overline{u}_g}{\partial z}+(\overline{\rho}_g\overline{v}_g+\overline{\rho'_g v'_g})\frac{\partial\overline{u}_g}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\mu_g\frac{\partial\overline{u}_g}{\partial r}-\overline{\rho}_g\overline{u'_g v'_g}\right)\right]-$$

$$-\frac{\partial\bar{p}}{\partial z}-\sum_i\bar{F}_{iz}+6\sum_j(\bar{\rho}_{gj}^{s}\bar{\alpha}_j^{s}-\bar{\rho}_g\bar{\alpha}_j)\bar{\beta}_j\delta_j^{-1}(\bar{u}_j-\bar{u}_g),\tag{7}$$

where the last term (additional, compared to Eq. (3) of [1]) includes the transition of the burnt carbon to the gas phase (i.e., the increase in the velocity of the carbon from that of the particles to that of the gas). A similar correction is also introduced into the equation of transfer of kinetic energy of turbulent gas fluctuations (7) of [1]:

$$\bar{\rho}_g\bar{u}_g\frac{\partial k_g}{\partial z}+(\bar{\rho}_g\bar{v}_g+\overline{\rho_g'v_g'})\frac{\partial k_g}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\times$$

$$\times\left\{r\left[\mu_g\frac{\partial k_g}{\partial r}-\frac{1}{2}\bar{\rho}_g\overline{v_g'(u_g'^2+v_g'^2+w_g'^2)}\right]\right\}-\bar{\rho}_g\overline{u_g'v_g'}\,\partial\bar{u}_g/\partial r-$$

$$-\bar{\rho}_g(\varepsilon+\varepsilon_p)+\Gamma_p-6\sum_j(\bar{\rho}_{gj}^{s}\bar{\alpha}_j^{s}-\bar{\rho}_g\bar{\alpha}_j)\bar{\beta}_j\delta_j^{-1}\times$$

$$\times(2k_g-\overline{u_g'u_j'}-\overline{v_g'v_j'}-\overline{w_g'w_j'})\tag{8}$$

(the last term in the right-hand side describes the expenditures of the fluctuation energy of the gas associated with the new compound).

Finally, the energy conservation equation will be given. For the particles of the i-th fraction

$$\rho_i\left[\bar{\beta}_i\bar{u}_i\frac{\partial c_i\bar{T}_i}{\partial z}+(\bar{\beta}_i\bar{v}_i+\overline{\beta_i'v_i'})\frac{\partial c_i\bar{T}_i}{\partial r}\right]=$$

$$=-\frac{\rho_i}{r}\frac{\partial}{\partial r}(rc_i\bar{\beta}_i\overline{v_i'T_i'})+6\bar{\beta}_i\delta_i^{-1}\left\{q_{\mathrm{conv}\,i}+q_{\mathrm{rad}\,i}+\right.$$

$$\left.+\,\omega_i\left[(\bar{K}_{1i}Q_{1i}+\bar{K}_{2i}Q_{2i})\bar{C}_{1i}^{s}-\bar{K}_{3i}Q_{3i}\bar{C}_{2i}^{s}\right]\right\}\tag{9}$$

(here $i=j,\ l$; $\omega_j=1$, $\omega_l=0$). In the right-hand side of Eq. (9) terms appear that describe turbulent heat transfer in the disperse phase, convective heat transfer between the gas and the particles, the radiative heat flux between the particles and the environment, and the thermal effect of chemical reactions (1) (for coke particles only). Similarly, the heat transfer equation for the gas is written as

$$\bar{\rho}_g\bar{u}_g\frac{\partial c_g\bar{T}_g}{\partial z}+(\bar{\rho}_g\bar{v}_g+\overline{\rho_g'v_g'})\frac{\partial c_g\bar{T}_g}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\times$$

$$\times\left[r\bar{\rho}_g\left(\frac{\nu_g}{\mathrm{Pr}}\frac{\partial c_g\bar{T}_g}{\partial r}-c_g\overline{v_g'T_g'}\right)\right]+\bar{u}_g\frac{\partial\bar{p}}{\partial z}+\sum_i\bar{F}_{iz}(\bar{u}_g-\bar{u}_i)-$$

$$-6\sum_i q_{ki}\bar{\beta}_i\delta_i^{-1}+6\sum_j(\bar{\rho}_{gj}^{s}\bar{\alpha}_j^{s}-\bar{\rho}_g\bar{\alpha}_j)\bar{\beta}_j\delta_j^{-1}\left[\bar{h}_j-\bar{h}_g+0.5(\bar{u}_g-\bar{u}_j)^2\right].\tag{10}$$

Equation (10) includes convective, molecular, and fluctuation transfer of the enthalpy of the gas flow, the work of the forces of pressure and interphase interaction, heat transfer between the gas and the particles, and the excess enthalpy and deficit of kinetic energy of that part of the matter of the coke particles that is transferred to the gas phase in reactions (1).

Integration of Eq. (4) over the cross section of the reactor, as was done in [1], gives

$$\frac{dG_g}{dz}=12\pi\int_0^R\sum_j(\bar{\rho}_{gj}^{s}\bar{\alpha}_j^{s}-\bar{\rho}_g\bar{\alpha}_j)\bar{\beta}_j\delta_j^{-1}\,rdr,\tag{11}$$

where the mass flow rate of the gas is $G_g = 2\pi \int\limits_0^R \bar{\rho}_g \bar{u}_g r dr$ (in [1] $G_g = \text{const}$). Thus, if the equation of state of the gas is taken into consideration, we obtain a closed system of equations consisting of: (3)-(6); (2) of [1]; (7); (4) and (5) of [1]; (8); (11) of [1]; (9)-(11) with unknown $\bar{C}_m$, $\bar{v}_g$, $\bar{\beta}_j$, $\bar{n}_j$, $\bar{\beta}_l$, $\bar{u}_g$, $\bar{u}_i$, $\bar{v}_i$, k_g, k_l, $\bar{T}_i$, $\bar{T}_g$, $\bar{\rho}_g$, $\bar{p}$, which can be solved by numerical methods. The correlations $\overline{C_m' v_g'}$, $\overline{n_j' v_j'}$, $\overline{v_i' T_i'}$, and $\overline{v_g' T_g'}$ appearing in Eqs. (3), (6), (9), and (10) are calculated by the gradient approach:

$$\overline{C_m' v_g'} = -D_t \frac{\partial \bar{C}_m}{\partial r}; \quad \overline{n_j' v_j'} = -D_j \frac{\partial \bar{n}_j}{\partial r};$$

$$\overline{v_g' T_g'} = -\frac{\nu_t}{\Pr_t} \frac{\partial \bar{T}_g}{\partial r}; \quad \overline{v_i' T_i'} = -(\nu_i/\Pr_i)\, \partial \bar{T}_i/\partial r \tag{12}$$

(ν_i and D_i are the coefficients of turbulent viscosity and diffusion of the "gas" of the i-th particles; ν_i is found from Eq. (22) of [2]; in the first approximation $D_i = \nu_i$, $\Pr_i = 1$). As was done in Eq. (21) in determining the correlations $\overline{u_g' u_j'}$ etc. in Eq. (8), it is necessary to include only the turbulent component of random motion of the particles; the results of [5] are used here. The other correlations of the fluctuation quantities are calculated in accordance with [1, 2].

Boundary conditions to Eqs. (4) and (5), (2) of [1], (7), (4) and (5) of [1], and (8) are prescribed as in [3]. By virtue of the symmetry of the problem, for the other equations on the axis of the reactor

$$\left(\frac{\partial \bar{C}_m}{\partial r}\right)_a = \left(\frac{\partial \bar{n}_j}{\partial r}\right)_a = \left(\frac{\partial \bar{T}_g}{\partial r}\right)_a = \left(\frac{\partial \bar{T}_i}{\partial r}\right)_a = 0.$$

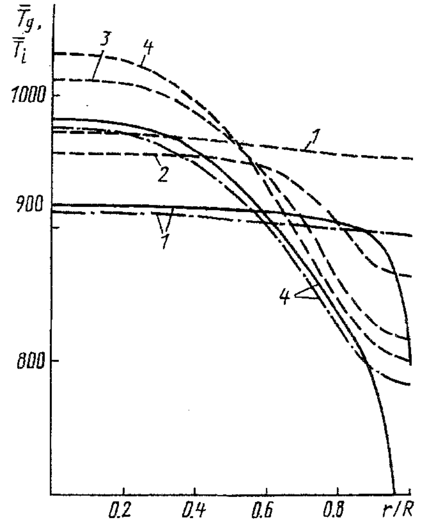
On the wall the condition of vanishing of the corresponding flow is used (cf. Eqs. (2) and (3) of [3]), then

$$\left[\frac{\partial (\bar{C}_m/\bar{\rho}_g)}{\partial r}\right]_w = \left(\frac{\partial \bar{n}_j}{\partial r}\right)_w = \left(\frac{\partial \bar{T}_i}{\partial r}\right)_w = 0.$$

For the temperature of the gas the condition of the first kind $\bar{T}_{gw} = T_w$ will be prescribed. As was done in [3], in the inlet cross section the flow is assumed to be uniform.

In Figs. 1–4 some results on motion, heat transfer, and combustion are presented for a coke-ash mixture in a channel with $R = 100$ mm. In the inlet cross section the averaged velocity of the gas $\bar{u}_{g0} = 6$ m/sec, the temperature of the phases $\bar{T}_{g0} = \bar{T}_{i0} = 900°\text{C}$, the concentration of oxygen $C_{10} = 0.21$, and the diameter of ash particles $\delta_l = 250\ \mu\text{m}$ were assumed. There versions differing in the total concentration of the disperse phase, the size of the coke particles, and the wall temperature were considered: case A, $\kappa = 1.1$, $\delta_j = 200\ \mu\text{m}$, $T_w = 800°\text{C}$; case B, $\kappa = 6$, $\delta_j = 200\ \mu\text{m}$, $T_w = 400°\text{C}$; case C, κ and T_w are the same but the coke particles consist of three fractions ($\delta_1 = 350\ \mu\text{m}$, $\delta_2 = 250\ \mu\text{m}$, and $\delta_3 = 150\ \mu\text{m}$) with equal weight concentrations. In all versions the concentration of coke is 0.1κ.

From Fig. 1 (here and in Figs. 2 and 4 solid lines show data for gas, dashed lines represent coke particles, and dash-dot lines are data for ash) it can be seen that the temperature of the coke exceeds that of the ash particles and the gas; this can be explained by heat release in heterogeneous chemical reactions (1). The temperature of the wall has a great effect on the temperature distribution and the burn-up efficiency. While in case A the function $T_j(r)$ is practically constant, case B is characterized by a substantial change in the temperature of the coke particles over the cross section of the apparatus, especially at large z. In particular, in the region $r/R \lesssim 0.675$ ($z = 7$ m) the heat generation exceeds the heat removal (convective and radiative) from the coke particles, which provides for efficient burn-up of them, the intensity of which increases toward the flow axis. Meanwhile, near the wall convective heat transfer becomes a decisive factor of the thermal state of the particles (due to a substantial increase in the temperature drop $\bar{T}_j - \bar{T}_g$), which results in cooling of the particles. From dashed lines 2, 3, and 4 it is possible to follow the evolution of the function $\bar{T}_j(r)$ along the flow. It can be seen that in the axial region the temperature of



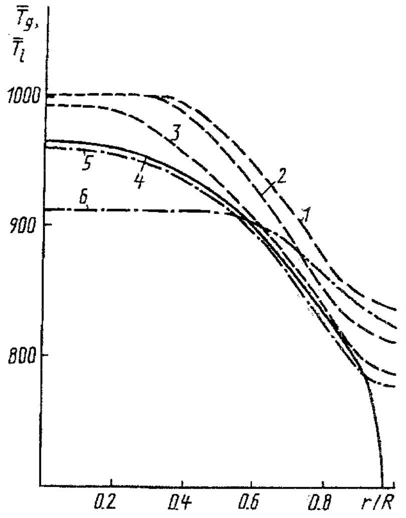
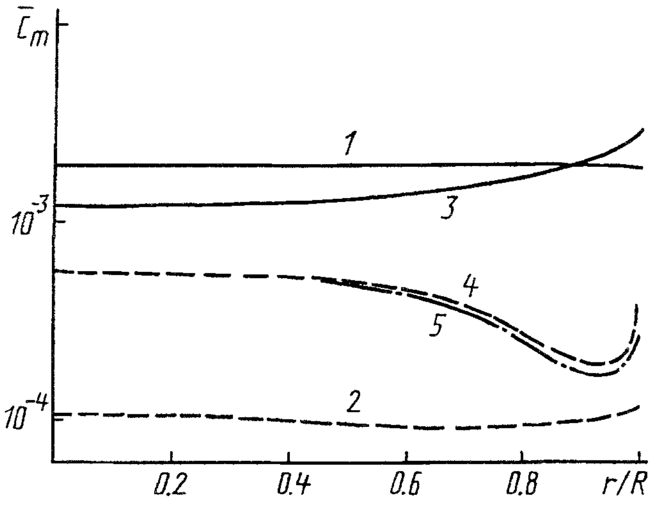


Fig. 1. Cross-sectional distributions of the temperatures of the phases: 1) case A, $z = 8.4$ m; 2–4) case B: 2) $z = 2.1$ m; 3) $z = 5.4$ m; 4) $z = 7$ m.

Fig. 2. Temperature field of the flow for case B: 1–5) $z = 7$ m; 1) $\delta_j = 350$ μm, 2) 250 μm, 3) 150 μm; 6) $z = 2.05$ m.



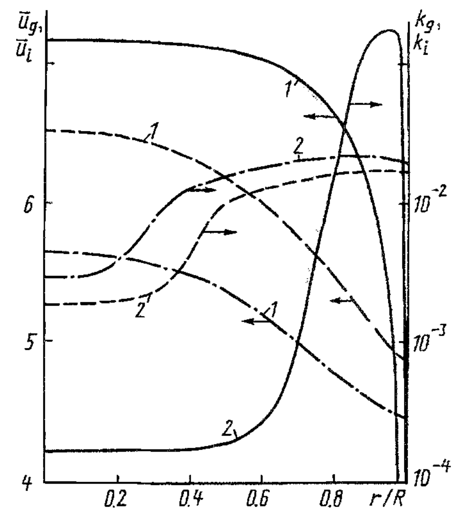


Fig. 3. Distribution of the concentration of the gas components: 1, 2) case A; 3–5) case B; 1, 3) oxygen; 2, 4) carbon dioxide gas; 5) carbon monoxide. C_m, kmole/m^3.

Fig. 4. Averaged longitudinal velocity (m/sec) (1) and fluctuation energy (m^2/sec^2) (2) for case A at $z = 8.4$ m.

the coke particles increases (the heat generation effect) and in the peripheral region it decreases (the heat transfer effect). It should be noted that in case A the maximum level of the process is lower than that in case B (in spite of a larger value of T_w), which is caused by the difference in the total reacting surface of the coke particles. In the flow core ($r/R \lesssim 0.85$ for case A and $r/R \lesssim 0.9$ for case B) the temperature of the ash particles is a little lower than the temperature of the gas; in the peripheral zone the difference $\bar{T}_g - \bar{T}_l$ changes sign and increases sharply as the distance from the wall decreases. This behavior of the function $\bar{T}_l(r)$ can be explained by intense mixing of particles due to the energy of their random motion (see below). This factor has a noticeable effect on the tempearture distribution of the coke particles too, especially in the peripheral zone.

Figure 2 illustrates the thermal state of the flow with the polydisperse particle composition. It is seen that at all points of a cross section, the temperature of the particles decreases as their size decreases. This is caused by the effect of convective heat exchange with the gas, which facilitates substantial cooling of the fine particle fractions. It should be noted that near the axis of the flow ($r/R \lesssim 0.32$), the temperatures of the large and medium coke particles are almost the same. This is caused, on the one hand, by intense burn-up and, on the other, by the effect of interparticle collisions on the residence time of particles of different fractions (see [4]).

It can be seen from Fig. 3 that the shape of the distribution of the concentration of the components depends strongly on the specifications of the calculation. In case A the functions $\overline{C}_m(r)$ are practically constant, which is caused by the high temperature of the wall. In case B the situation is different. In the region $r/R \lesssim 0.94$ the concentrations of CO and CO_2 decrease monotonically with increase in r due to a decrease in the rate of reactions (1) that is related to the temperature of the coke particles (see Fig. 1). Meanwhile, near the wall the values of $\overline{C}_2$ and $\overline{C}_3$ increase sharply – the increase in the density of the gas appears to be more important here.

In Fig. 4 the distribution of kinematic characteristics of the flow is shown. In general, the curves $\overline{u}_g(r)$ and $\overline{u}_i(r)$ are similar to the results for an isothermal flow given in [3]: in the core of the flow the higher the free-fall velocity of the particles, the more they lag behind the gas; in the near-wall region the particles are ahead of the gas since the drag force is negative here and suspension of the particles is mainly determined by their random motion. Meanwhile, unlike [3], in Fig. 4 the distribution of the gas velocity is somewhat less filled and the points of intersection of the curves $\overline{u}_g(r)$ and $\overline{u}_i(r)$ are shifted toward the axis of the reactor. It should also be noted that in the region $r/R < 0.8$ the energy of random motion of the particles greatly (by more than an order of magnitude near the axis) exceeds the fluctuation energy of the gas and this confirms the conclusion made in [3] about the dominant role of pseudoturbulent transfer in the mechanics of particle motion. It is seen from Fig. 4 that (unlike the results of [3] and cases B and C, where $\kappa = 6$) at a relatively low concentration of disperse material, the random motion of the heavier particles is more intense. An analysis of the balance of the terms in the equation of transfer of fluctuation energy (11) of [1] (see also Eqs. (13), (14), (19)-(21) in [2]) shows that in this case collisions with particles of "their own" fraction and the effect of the drag force are the main factors responsible for generation and dissipation. It should be noted that the rate of dissipation of the energy of random motion due to interaction with the gas (see Eq. (21) in [2]) depends strongly on the size and density of the particles, and therefore for coke particles the value of k_i is slightly lower than that for ash.

NOTATION

Q, thermal effect of the reaction; ρ, density; C_m, C^s_{mj}, concentration of the m-th component of the gas inside and on the surface of a particle of the j-th fraction; M, molecular weight; z, r, cylindrical coordinates; u, v, w, axial, radial, and transverse components of the velocity; δ, particle size; β, true volume concentration of the particles; a_{mj}, coefficient of diffusion mass transfer of particles j with the m-th component of the gas; K_{1j}, K_{2j}, K_{3j}, rates of heterogeneous reactions (1) for particles j; n, number concentration of the particles; k, kinetic energy of fluctuation motion; h, enthalpy; μ, ν, dynamic and kinematic viscosities; p, pressure; F, force of interphase interaction; ε, rate of viscous dissipation of turbulent energy; Γ_p, ε_p, rates of generation and dissipation of turbulent energy due to the effect of the particles; c, specific heat; T, temperature; Pr, Prandtl number; R, reactor radius; D, diffusion coefficient; k, mass flow rate concentration. Subscripts: a, flow axis; g, p, gas and particles; i, j, l, number of a fraction; m, number of a gas component; t, turbulent analog; w, wall; 0, inlet cross section; $\overline{\ }$, $'$, averaged and fluctuation components.

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