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An Investigation of Dynamics of Oxygen Burning Out of Lift-reactors and Pecular Features of Gas Flowing Through a Layer of Immovable Catalyzer

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Abstract. The work presents a mathematical model of the flow of dispersed particles accelerated with a stream of reacting gas in the two-dimensional domain. The model provides to take into account interactions of gas streams and the dispersed phase. Computerized experiments have allowed to find the areas for fuel gas to be injected in order to maximize the rate of oxygen burning out of catalyzer pores. Special features of gas flowing through a layer of immovable built-in porous medium are studied, these being determined by surface deformation of the layer. From the practical point of view the solution of the problem is closely related to theoretical calculations and optimization of the processes in lift-reactors and reactors with a layer of immovable catalyzer.

1 Introduction

Investigations into dynamics of the flow of dispersed particles are of much interest for calculating catalytic reactors with a layer of moving catalyzer. One of the designs of such units is a lift-reactor, with a fine-dispersed catalyzer fed into the reaction zone and accelerated with a gas stream (Fig. 1). The absence of symmetry in the distribution pattern of the stream sets up prerequisites for the problem to arise in connection with proportional intermixing at the bottom of the reactor. This problem is of special significance if one takes the reagent as an accelerating gas to prepare a gas/particles mixture for the principal reaction; for example, when in order to suppress phenol formed during the catalytic cracking process, it is necessary to burn oxygen out of gas mixture fed into the reaction zone together with the catalyzer, by means of propane in the stream of accelerating gas. Efficient intermixing can be realized at the expense of rational arrangement of the areas of gas injection. Considering that gas injection is performed through the walls of the reactor reservoir, the control over the adjacent flow is extremely important in optimizing the design features of the most different chemical reactors. As a design modification it is possible to apply surface deformation of a layer of porous medium to favour intermixing among gas components to the best.

The present paper is aimed at mathematically simulating a dispersed catalyzer flowing in the riser of a lift-reactor and at determining the areas of combustible gas to be injected so that to ensure the greatest possible oxygen burn-out in the reactor operating zone. Among the aims is also the investigation of some peculiar features of gas flowing through a layer of immovable catalyzer.

The mathematical model of the flow of the reacting gas mixed with dispersed catalyzer is based upon equations of dynamics of continuous media (Nigmatulin, 1990). Since the flow of the dispersed phase at the initial stage occurs with the interaction of particles with each other, a necessity has arisen to take this interaction into account in the model. It seems worthwhile to draw on the concepts presented by Savage (Savage, 1979).

2 A Mathematical Modelling of a Fine-Dispersed Catalyzer Flowing along the Channel

Let us consider a flow of the two-phase gas/fine-dispersed catalyzer mixture at the bottom of a lift-reactor, with acceleration of the catalyzer up to the transportation regime at the expense of gas injection (Fig. 1). As the catalyzer enters the operating zone on leaving the regeneration chamber, its temperature will be high enough ($\sim 650\,^{\circ}$C). Due to high heat capacity of the catalyzer and its considerable content by mass, the temperature of the injected gas becomes equal rapidly to that of the catalyzer. Thus, there is a reason to think that the conditions of the process are isothermic. Filtration heating and heat realease in the course of subsidiary chemical reactions are neglected.

Let us assume that a gas stream containing solid particles corresponds to the hypotheses of dynamics of multiphase media (Nigmatulin, 1990) with regard both

(a) (b)

Figure 1: Scheme of operating domain of the lift-reactor (a); catalyser concentration field at ordinary gas injection (b).

to interphase forces and interaction of the particles. In this case the behavior of interphase forces is supposed to be conditioned by the state of velocity nonequilibrium at sufficiently slow flows determined by Stokes' frictional force.

Interaction among particles in a dense flow of the dispersed phase suggests such medium to be a collision one. Pursuing a goal of practical results and ignoring the deformational peculiar features of granular media, let us take up a simplified formulation of the problem on the flow of dispersed medium, when components of the given stress tensor, that is responsible for contact pulse transmission among particles, are determined only by the deviator of deformational velocities, with the dependence between viscosity coefficient and solid phase content by volume taken into account (Savage, 1979).

The solution of the problem in the two-dimensional domain requires boundary conditions to be laid down properly. It is necessary to note in this connection that the assumption accepted in dynamics of multiphase media on the dominating role of dispersed phase viscosity in the forces of phase interaction as compared to their action under shear deformations should not lead to ignoring tangential stresses in the same phase. This conclusion is based on the necessity to interpret the boundary conditions and their influence upon the method of solving the problem in physical terms.

Relying on the given arguments, let us write a system of equations for the process under investigation:

$$\frac{\partial \rho_i}{\partial t} + \nabla \rho_i \vec{v}_i = 0\,, \qquad (1)$$

$$\begin{aligned}\frac{\partial \rho_i v_i}{\partial t} + \nabla \rho_i v_i |\vec{v}_i| &= \\ &= -\alpha_i \operatorname{grad} p + \mu_i \Delta \vec{v}_i + \vec{F}_{ij} - \rho_i \vec{g}\,,\end{aligned} \qquad (2)$$

where

ρ_i is the density of the i-th phase averaged by space, kg·m^{-3};

a_i is the content of the i-th phase by volume;

$\vec{v}_i$ is the velocity vector of the i-th phase, m·s^{-1};

p is the dispersive phase pressure, kg·m^{-1}·s^{-2};

μ_i is the phase dynamical viscosities, kg·m^{-1}·s^{-1};

$\vec{F}_{ij}$ is the vector of phase interaction forces, kg·m^{-3};

$\vec{g}$ is the free fall acceleration, kg/m^{-2}·s^{-2}.

The equation of state for the dispersive phase is as follows:

$$p = \rho_1^0 R T_c \qquad (T_c = \text{const})\,, \qquad (3)$$

where

ρ_1^0 is the true density of the 1st phase, kg·m^{-3};

R is the gas constant for the given gas mixture, m^2·s^{-2}·K^{-1};

T_c is the temperature in the reactor, K.

The following relationships are added:

$$\rho_i = \alpha_i \rho_i^0\,; \qquad a_1 + a_2 = 1\,. \qquad (4)$$

Expressions for phase interaction forces are taken in the form:

$$\vec{F}_{ij} = -\vec{F}_{ji} = \eta_\mu \alpha_i \alpha_j a^{-2} (\vec{v}_i - \vec{v}_j)\,; \qquad (5)$$

where

η_μ is the structural ratio;

a is the diameter of particles in the dispersed phase, m.

Besides, let us treat the law of variations in viscosity of a dispersed phase in terms of the formula put forward by Savage (Savage, 1979) and on the basis of Bagnold's experiments:

$$\mu_2 = \beta \left(\frac{\alpha_{2*} - \alpha_{20}}{\alpha_{2*} - \alpha_2} \right)\,, \quad \alpha_{20} < \alpha_2 < \alpha_{2*}\,;$$

where

β is the empirical ratio;

a_{2*} is the greatest possible concentration of the dispersed phase;

a_{20} is the least concentration required for “fluidity” of the dispersed phase.

In combination with formulae (5) and (6) the system of equations (1)–(4) makes up a closed model of fine-grained catalyzer flowing. This system has been numerically realized by means of a computer code based on the modified Finite Volume Method, with the SIMPLE algorithm applied.

Boundary conditions correspond to the design illustrated in Fig. 1(a).

$$\vec{v}_i\Big|_{(inp)} = \vec{v}_{(inp)}\,, \qquad \vec{v}_i\Big|_{(inj)} = \vec{v}_{(inj)}\,,$$

$$\vec{v}_1\Big|_{(wall)} = 0\,, \qquad \frac{\partial \vec{v}_2}{\partial y}\Big|_{(wall)} = 0\,,$$

$$p\Big|_{(out)} = p_{(out)}\,,$$

$$\alpha_1\Big|_{(inp)} = \alpha_{(inp)}\,, \qquad \alpha_1\Big|_{(inj)} = \alpha_{(inj)}\,.$$

Figure 1(b) shows the result of calculating the field of the dispersed phase concentration and attests to irregular distribution of the catalyzer over the zone of the reactor chamber under discussion.

3 Calculations of Oxygen Concentration

Catalyzer is supplied into the reactor chamber on leaving the regeneration zone, and, as special investigations show, there is a gas mixture with remaining oxygen among other components. Since a lift-reactor may be used in catalytic cracking process, this oxygen may result in forming phenol and subsequently dioxins unwanted from the environmental standpoint.

For the remaining oxygen to be removed off the zone of principal chemical reactions most efficiently, it has been suggested that oxygen should be burnt out at the stage of accelerating the catalyzer at the bottom the lift-reactor chamber by injecting combustible and accelerating gases in combination. It has been also taken into account that this combustible gas and its products are neutral both for the efficiency of catalytic cracking process and catalyzer activity.

In view of oxygen considerably small initial concentration and heat moderate total input because of oxidation reaction, let us consider the process of burning out oxygen in the context of the mathematical model described above with additional equations to determine concentrations of the given components of the gas mixture:

$$\frac{\partial c_m \rho_1}{\partial t} + \nabla c_m \rho_1 \vec{v}_1 = \mathcal{J}_m\,,$$

where

$m = 1$ corresponds to oxygen, and $m = 2$ corresponds to combustible gas;

$\mathcal{J}_m = \mathcal{J}(c_1, c_2, T)$ is the intensity of the chemical reaction.

Figure 2(a) presents the calculating data for oxygen concentrations at normal gas injection. It is evident that in this case oxygen does not completely burn out of the zone in question, that being associated with catalyzer irregular distribution. Numerical experiments have allowed to find the best mode of injecting combustible gas at fixed consumption. The associated field of oxygen concentrations is shown in Fig. 2(b).

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(a) (b)

Figure 2: Oxygen concentration field at ordinary gas injection (a) and after optimization (b).

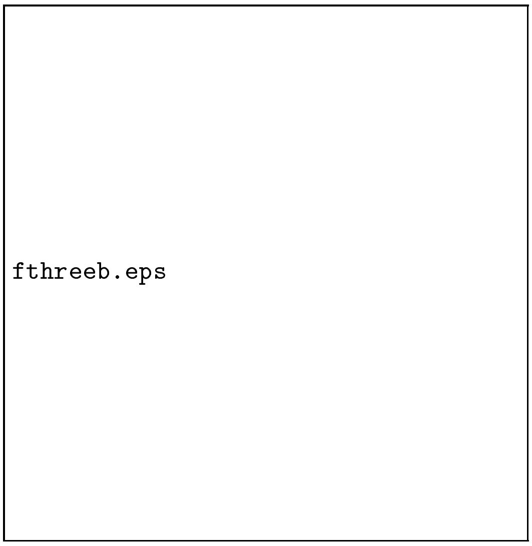
4 The Investigation into Peculiar Features of Gas Flowing through a Layer of Immovable Catalyzer

It is known from the literature about the effect related to the passage of gas through a layer of porous or granulated medium, which is called the effect of "hare ears". This effect makes itself evident in the formation of a macroscopic ear-like heterogeneity of the velocity field behind the porous layer. Opinions differed on how to explain this phenomenon, for instance, by variations in porosity just near the wall or by the deformational pattern of a porous medium. Based on the experimental investigations, Goldshtik (1984) found out that the "hare ears" effect owed its origin to surface deformations of a porous medium.

The above given model has suggested to make some numerical investigations of this phenomenon. In doing so, the velocity of particles of the dispersed medium is assumed to be zero ($\vec{v}_2 = 0$), and the medium occupies a portion of the channel as displayed in Fig. 3(a). Besides, it is assumed that $\alpha_2 =$ const.

Figure 3(b) shows the calculated gas horizontal velocity in sections (1) and (2), where the "hare ears" effect is clearly displayed. For comparison purposes

(a)



(b)

Figure 3: Scheme of the channel with a porous layer (a); velocity distribution of the gas flow on cross-sections 1 and 2 (b); line 3 corresponds to plane layer surface.

line (3) is given in Fig. 3(b), that corresponds to the plane s urface of the porous layer. Thus, one should conclude that it is precisely the outer surface deformation of the laeyr that is responsible for the effect to be revealed. It should also be mentioned that the shape of deformation makes no special difference. The only important thing that the surface of the porous medium must form an acute angle ($\varphi < \pi/2$) with the wall of the channel.

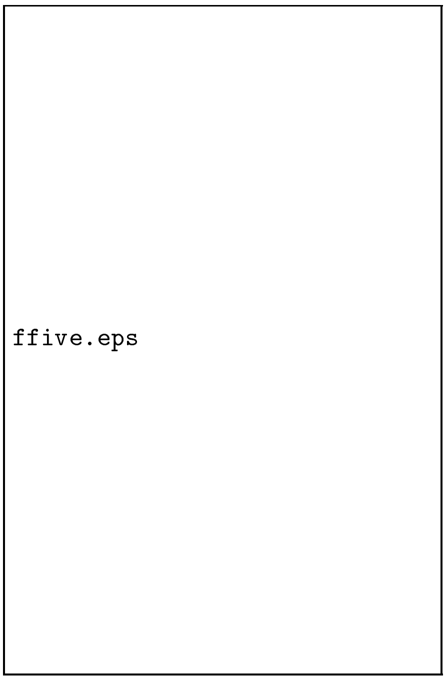


Figure 4: Fields of velocities vectors (arrows) and that of gas pressure in channel (correspond to the scheme in Fig. 3(a).

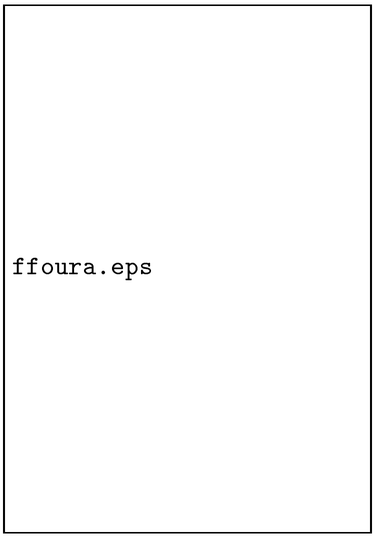
A comparison of the pressure field (Fig. 4) with the vector field of velocities shows it most clearly that the direction in velocity under flowing is perpendicular to pressure isolines.

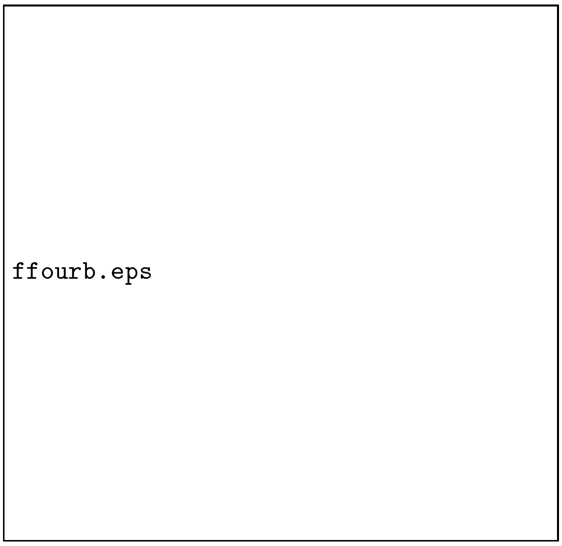
Thus, the “hare ears” effect arises from cumulation of the flow with a jet stream formed near the wall. This is also evidenced by calculations made for porous layers with the reverse deformation (Fig. 5(a)). In Fig. 5(b) a jump in horizontal velocity is clearly seen in sections (1) and (2) in the central portion of the channel with the formation of a single jet.

5 Conclusion

The present paper is an attempt to describe a fine-grained catalyzer flowing along the lift-reactor channel within the region of acceleration and to determine the pattern in the course of chemical reaction depending on reagent supplying conditions. A possibility is shown on the basis of the given mathematical model to optimize the arrangement of combustible gas injection zones and to efficiently remove a gas component unwanted in the process, namely, oxygen.

The investigation into peculiar features of a gas flow behind the catalyzer immovable layer has resulted in a clear-cut interpretation of the “hare ears” effect. This effect is determined to correlate with gas flow cumulation near the wall and to depend on the value of the angle formed between the outer surface of a catalyzer layer (or a porous medium in general) and the wall of the channel.





(a) (b)

Figure 5: Scheme of the channel with a V-shaped porous layer (a); distribution of gas flow velocity in cross-sections 1 and 2 (b).

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