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Catalysis Today 24 (1995) 297–298

CATALYSIS TODAY

Numerical modelling of the dynamics of methane oxidation

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Abstract

The dynamics of burning gas extraction from hard particles and their burning are considered. The level of mathematics modelling of physical and chemical processes, is on the basis of separate hard fuel particles and gaseous volume.

1. Physical settings of the problem

Polydispersed fuel solid particles with dimensions which varied from 3 to 1000 mkm, moisture – 4–30%, with the initial speed 0 m/sec, are introduced to the high-temperature gaseous flow ($T_g^0 = 1000$–2000 K, $Re_g = 10^4$–10^7); there is free oxygen (O_2) and coupling oxidizer (H_2O). During running and heating of coal particles there occur fluently going processes of the appearance of gaseous hydrocarbons CH_4, C_2H_2, nitrogenous substances HCN, NH_3, and the burning reaction – carbon–hydrogen remains gasification. While obtaining a mathematical description of dynamics of hard fuel particles burning and burning gas, the common suppositions of many-phase aerodynamics [1] are used. The elemental composition of hard particles: $A^c = 10\%$; $V^{daf} = 48.0$; $C^{daf} = 71\%$; $H^{daf} = 4.9\%$; $O^{daf} = 23.1\%$; $N^{daf} = 0.7\%$; $S\Sigma = 0.3\%$

2. The mathematical model

The mathematical description of dynamics of drying processes, pyrolysis and nonstationary temperature field in separate coal particles is drawn from the laws of mass and energy conservation, so this description has the next type:

$$\frac{\partial \Phi_i}{\partial \tau} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_i r^2 \frac{\partial \Phi_i}{\partial r} - \Phi_i r^2 V_i\right) - G(\tau, r) \qquad (1)$$

where Φ_i – concentration (temperature); D_i – diffusion coefficient (neat conductivity); τ – time; $G(\tau,r)$ – the speed of the phase transfer; V_i – the speed of filtration. In the gaseous phase one solved the equations of chemical kinetics of burning and formation of poison substances for the environment (NO_x) from the first compounds (NH_3 and HCN). As a basic model of chemical transformation kinetics in the gaseous phase the next model is adopted [2]:

$$CO + \tfrac{1}{2}O_2 \rightleftharpoons CO_2, \qquad CH_4 + \tfrac{1}{2}O_2 \rightarrow CO + 2H_2,$$
$$NH_3 + O_2 \rightarrow NO + H_2O + \tfrac{1}{2}H_2, \qquad NH_3 + NO \rightarrow N_2 + H_2O + \tfrac{1}{2}H_2,$$
$$N_2 + O_2 \rightleftharpoons 2NO, \qquad HCN + H_2O \rightarrow NH_3 + CO,$$
$$NO + CH_4 \rightarrow HCN + H_2O + \tfrac{1}{2}H_2, \qquad H_2 + \tfrac{1}{2}O_2 \rightleftharpoons H_2O$$

The equations of chemical kinetics corresponding to this scheme has the next type:

$$\dot{x} = \Sigma \gamma_s W_s(x,T) \qquad (2)$$

SSDI 0920-5861(95)00048-8

where x – calculational concentration vector, γ_s – s-stage stereometric vector, w_s – s-stage speed. For closing the system, describing physical and chemical processes in the two-phase flow, the mathematical description of one-dimensional stream reactor [3] was used.

3. The computing experiment

Differential Eq. (1) with critical conditions of III kind have been solved using integro-interpolation method. The non-explicit conservative difference schemes with the convective element are constructed using characteristic method. We obtained schemes that approximate initial differential equations with the first accuracy order according the time and space. This schemes are stable for parameters, known from experience. while solving the system of differential Eq. (2) the methods of hard system numerical solution were used.

The process of coal dust gasification is complex, this process depends on some factors (temperature and fuel moisture). The whole computations series of coal processing dynamics have been performed (for different values of technological parameters). It has found out, that coal pyrolysis and drying dynamics features at high speed heating is pressure gradient presence in porosite fuel particles. This is one of reasons, causing its decomposition. The characteristic time intervals were obtained for each polyfractional coal loading, which may be used during designing the rational scheme of fuel preparation. As the result of mathematical modelling we received all the stages of mechanism formation's the nitric oxide in combustion processes and distribution graphics of heat, concentration's fields of gaseous volume.

4. References

[1] E.S. Oran, J.P. Boris, Numerical Simulation of Reactor Flow, Elsevier, New York, 1987.
[2] V.I. Chmyrov, V.O. Krol, A.K. Sklyambaeva, Fiz. Goreniya Vzryva, 1993, N 4.
[3] R. Aris, Introduction to the Analysis of Chemical Reactors, Chemistry, Moscow, 1967.