EFFECTS OF REAGENT CONSUMPTION AND HEAT LOSS IN IGNITION IN A VESSEL

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Two approximate analytical methods are widely used in research on thermal ignition: the stationary theory [1] and the nonstationary one [2]. The first predicts the critical explosion conditions very closely. Direct numerical integration has been used [3] to obtain a solution for thermal ignition, which indicated that ignition near the heated walls can accompany ignition at the center. The difference between the critical conditions for ignition at the wall and self-ignition can be defined only from the interaction between the initial and boundary conditions. The extent of combustion is substantial in both cases [1], and it subsequently plays a substantial part in setting up the temperature conditions in the vessel. A study is made here of the thermal decomposition of methyl nitrate vapor, which incorporates the diffusion and finite reaction rate. Monte Carlo simulation is used with a planar electrically conducting medium [4].

Consider a plane-parallel vessel with unbounded walls filled with methyl nitrate vapor.

The problem is put in the form

$$\mathrm{Fo} > 0, \quad 0 < X < 1, \tag{1}$$

$$\frac{\partial\theta}{\partial\,\mathrm{Fo}} = \frac{\partial^2\theta}{\partial X^2} + \eta\delta\exp\left(\frac{\theta}{1+u\theta}\right),$$

$$\frac{\partial\eta}{\partial\,\mathrm{Fo}} = \mathrm{Le}\,\frac{\partial\eta}{\partial X^2} - \eta\delta\sigma\exp\left(\frac{\theta}{1+u\theta}\right);$$

$$\mathrm{Fo} = 0, \quad 0 \leqslant X \leqslant 1, \quad \theta = 0, \quad \eta = 1;$$

$$\mathrm{Fo} > 0, \quad X = 0, \quad \frac{\partial\theta}{\partial X} = 0, \quad \frac{\partial\eta}{\partial X} = 0;$$

$$\mathrm{Fo} > 0, \quad X = 1,$$

$$-\frac{\partial\theta}{\partial X} = \mathrm{Bi}\,(\theta - \theta_w), \quad \frac{\partial\eta}{\partial X} = 0, \tag{2}$$

where $\theta = \frac{E}{RT_0^2}(T - T_0); \quad \eta = \frac{c}{c_0};$

$$\delta = \frac{E}{RT_0^2}\,\frac{Q_p}{\lambda}\,l^2k_0c_0 \times \exp\left(-\frac{E}{RT_0}\right); \quad \mathrm{Bi} = \frac{\alpha}{\lambda}\,l;$$

$$\sigma = \frac{RT_0^2}{E}\,\frac{c_v\rho}{Q_pc_0}; \quad \mathrm{Le} = \frac{D}{a}; \quad u = \frac{RT_0}{E};$$

$$X = x/l; \quad \mathrm{Fo} = at/l^2,$$

The symbols Bi, Fo, and Le are, respectively, the Biot, Fourier, and Lewis numbers, while E is the activation energy, Q_p is the heat of reaction T_0 is the initial temperature, which equals the wall temperature T_W, c_0 is the initial concentration, k_0 is the preexponential factor, R is the universal gas constant, l is the transverse size of the vessel, and λ, c_v, a, D, ρ, α are, respectively, the thermal conductivity, specific heat, thermal diffusivity, diffusion constant, density, and heat-transfer coefficient.

The kinetic data on the decomposition of methyl nitrate vapor were taken from [5].

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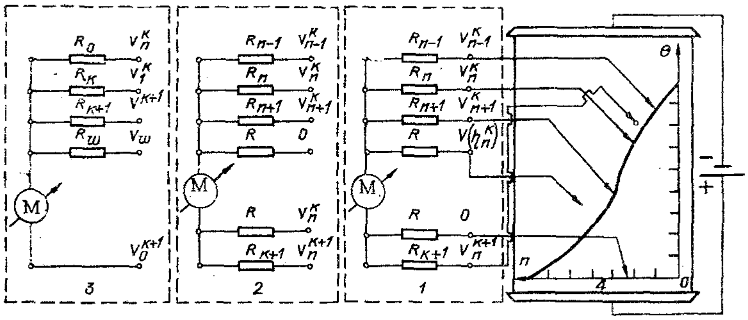

Fig. 1

The initial problem of (1)-(2) was approximated via the following difference equations:

$$\theta_n^{k+1} = \frac{\Delta \mathrm{Fo}}{\Delta X^2}\left(\theta_{n+1}{}^k + \theta_{n-1}{}^k\right) + \left(1 - 2\frac{\Delta \mathrm{Fo}}{\Delta X^2}\right)\theta_n{}^k + \eta_n{}^k\,\delta\Delta\,\mathrm{Fo}\exp\left(\frac{\theta_n{}^k}{1+u\theta_n{}^k}\right); \tag{3}$$

$$\eta_n{}^{k+1} = \frac{\Delta \mathrm{Fo}}{\Delta X^2}\left(\eta_{n+1}{}^k + \eta_{n-1}{}^k\right) + \left[1 - 2\frac{\Delta \mathrm{Fo}}{\Delta X^2} - \delta\sigma\Delta\,\mathrm{Fo}\exp\left(\frac{\theta_n{}^k}{1+u\theta_n{}^k}\right)\right]\eta_n{}^k,$$

$$(n = 1, \ldots, N-1;\ k = 1, 2 \ldots);$$

$$\theta_n{}^0 = 0,\ \eta_n{}^0 = 1,\ \theta_0{}^{k+1} = \theta_1{}^{k+1},\ \eta_0{}^{k+1} = \eta_1{}^{k+1},$$

$$\theta_N{}^{k+1} = \frac{\theta_{N-1}{}^{k+1} + \theta_{N-1}{}^k + 2\mathrm{Bi}\,\Delta X\theta_w + (M - 1 - \mathrm{Bi}\,\Delta X)\,\theta_N{}^k}{1 + M + \mathrm{Bi}\Delta X}, \tag{4}$$

$$\eta_n{}^{k+1} = \eta_{N-1}{}^{k+1}.$$

The stability conditions for (3) are

$$\frac{1}{M} = \frac{\Delta \mathrm{Fo}}{\Delta X^2} \leqslant \frac{1}{2}; \tag{5}$$

$$1 - 2\frac{\Delta \mathrm{Fo}}{\Delta X^2} - \delta\sigma\Delta\,\mathrm{Fo}\exp\left(\frac{\theta_n{}^k}{1+u\theta_n{}^k}\right) > 0. \tag{6}$$

Condition (6) was used in the calculations, which is more restrictive than (5) as regards the parameters of ΔFo and ΔX.

To meet (6) during the calculations with a given ΔX one had to reduce ΔFo in accordance with the increase in reaction rate.

One transfers from (2) to (4) by the method of elementary heat balances [6].

Before the start of solution, the arithmetic section was programmed structurally in accordance with the difference scheme [4] (Fig. 1), with 1-3 as decision elements for the integration of (3) and (4). The values of the resistors were taken as

$$R_{n-1} = R_{n+1} = 1,\quad R_n = \frac{1}{M-2},\quad R_{k+1} = \frac{1}{M}, \tag{1}$$

$$R = \frac{1}{\delta\Delta X^2 \exp\left(\dfrac{\theta_n{}^k}{1+u\theta_n{}^k}\right)};$$

$$R_{n-1} = R_{n+1} = 1;\quad R_n = \frac{1}{M-2};\quad R_{k+1} = \frac{1}{M}; \tag{2}$$

$$R = \frac{1}{\delta\sigma\Delta\,X^2 \exp\left(\dfrac{\theta_n{}^k}{1+u\theta_n{}^k}\right)};$$

$$R_k = R_{k+1} = 1;\quad R_0 = \frac{1}{M - 1 - \mathrm{Bi}\,\Delta X}; \tag{3}$$

$$R_w = \frac{1}{2\,\mathrm{Bi}\,\Delta X}.$$

The step in the time coordinate was adjusted via R_n, R_{k+1}, R_0.

A planar electrically conducting medium (Fig. 1, part 4) enabled us to solve the problem directly in graphical form without intermediate recordings.

Figure 2 shows the nonstationary temperature distributions and concentrations (curves 1-6 correspond to Fo = 0.025, 0.0625, 0.07, 0.0710, 0.07125, 0.07142), while Fig. 3 shows the nonstationary reaction-rate distribution (curves 1-6 correspond to Fo = 0.06746, 0.06764, 0.06814, 0.06912, 0.07066, 0.07299) for values of the parameter $\delta = 17.0688$, $\sigma = 0.0574$, $\mathrm{Bi} = 4.8$, $\theta_w = 0$; for comparison, Fig. 2 shows (broken line) the temperature distribution for adiabatic combustion (Fo = 0.07 and Fo = 0.07142), which resembles the temperature and concentration distributions:

$$\theta(X) = \frac{1}{\sigma}[1 - \eta(X)].$$

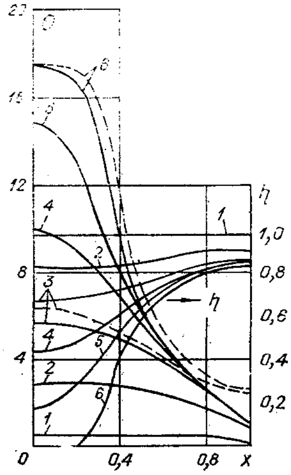

Fig. 2

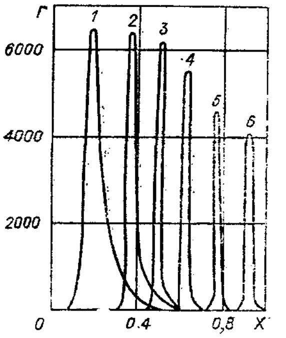

Fig. 3

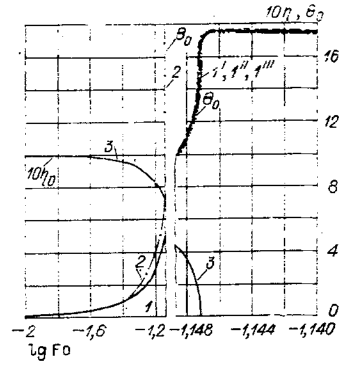

Fig. 4

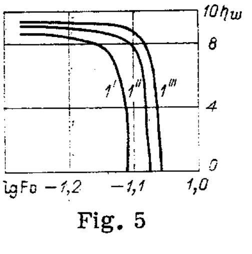

Fig. 5

Comparison of the curves shows that the heat transfer disrupts the similarity. The discrepancy is largest near the walls of the vessel, because the heat transfer to the surroundings lowers the temperature there, and the reaction rate is dependent exponentially on the temperature, so the decomposition at the center is more rapid than that at the walls (Fig. 2). Then the region of burnup expands (Fig. 3).

Figure 4 shows the temperature and concentration distributions over the axis of the vessel as functions of time (1 and 3). Within the working time interval, the temperature θ_0 rises only to some maximum value θ_{om} (calculations show that θ_{om} corresponds to T_m, which coincides with the theoretical possible adiabatic combustion temperature):

$$T_m \doteq T|_{t=0} + \frac{Q_p}{c_v}.$$

The temperature at the axis $\theta_0(\log \mathrm{Fo})$ was compared with the analogous relationship neglecting the consumption (curve 2). It is clear that the difference between the curves is initially inappreciable (burnup slight, Fig. 4); subsequently, curve 2, which describes the effect of thermal explosion, lies above curve 1, which corresponds to higher temperatures. From a certain instant onwards, the temperature rises exponentially (an analogous solution was obtained in [3] for a cylindrical layer of material), and the difference between 1 and 2 becomes very great. Figure 5 illustrates the concentration variation at the vessel walls as a function of time in relation to the heat-transfer conditions (Bi). Figure 4 implies that the ignition time is not dependent on Bi. The total burnup time, during which the initial material vanishes, increases somewhat as the heat transfer to the environment increases (Fig. 5). Curves 1'-1''' relate to Bi of 0, 4.8, and infinity, respectively. Incorporation of the consumption allows one to determine the total combustion time and to trace the formation of the flame. The concentration remains virtually constant during the ignition, so one expects that the burnup will not alter the critical ignition limits. As the density and pressure vary with temperature on account of free convection in the gas [7], there is a certain change in the temperature and concentration distributions, but there is no qualitative difference from our results.

This simulation method with a conducting medium can be used in handling combustion-theory problems and gives adequate accuracy (0.5-1%) for the process.

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