MODES OF INFILTRATION BURNING IN A POROUS CONDENSED

SYSTEM WITH REPEATED REACTION WAVES

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Various modes of infiltration burning are considered for porous condensed systems with multiple reaction-wave passage. These states are optimized for various organization schemes.

When infiltration burning is used in organizing some technological process [1], one naturally has to consider the productivity, which is determined by the reaction-wave speed through the condensed phase.

If the reaction is retarded by the product, it is desirable to examine not only onewave states [2-7] but also ones with multiple wave passage (multiwave states).

These are of interest because if one defines the reaction temperature level T_c and the final extent of conversion $\eta_f(\lim \eta_f = 1)$ for the one-wave state, this unambiguously determines not only the input parameters (the independent ones) such as the gas-mixture infiltration rate v_0 and the concentration c_1^0 of the oxidant but also the output parameter: the reaction-wave propagation speed u_1 [5, 6]. The situation is different in a multiwave state, which involves multiple wave passage at a given temperature T_c but with successively varying extents of reaction in the ranges $0-\eta_{f1}$, $\eta_{f1}-\eta_{f2}$, ..., $\eta_f(N_{-1})-\eta_{fN} \equiv \eta_f$, where N is the number of waves. In this case, it is possible to vary the number of waves and the conversion intervals for each of them, which in turn opens up the scope for optimizing the throughput, which is determined by the obvious relation

$$u_{N} = \frac{u_{N1} u_{N2} \dots u_{NN}}{u_{N2} u_{N3} \dots u_{NN} + u_{N1} u_{N3} \dots u_{NN} + \dots + u_{N1} u_{N2} \dots u_{N(N-1)}},$$
 (1)

where u_{Nj} is the speed of wave j in the N-wave state, which is determined, as noted above, by specifying T_c and by the choice of the input parameters v_{oj} and c_{ij}^0 .

The condition for constancy of the combustion temperature for the entire wave sequence is natural for a process in which the reaction temperature is limited by reference to the yield of the target product, and it is shown below that this enables one in a fairly simple fashion to derive an expression for the performance characteristics of the multiwave state.

To examine the trends in such modes of combustion, we derive an expression for the wave speed for an exothermic reaction in the case of a nonzero initial extent of reaction η_0 .

The system of equations for the heat and mass transfer and the chemical kinetics is similar to that used previously [4-7] and describes the wave process in a coordinate system moving with the reaction wave:

$$\frac{d}{dx} \left[(c_1h_1 + c_2h_2) v - s (c_3h_3 + c_4h_4) u \right] = \frac{d}{dx} \left[\lambda(\eta) \frac{dT}{dx} \right] - Qc_3^0 u \frac{d\eta^*}{dx},$$
(2)

$$\frac{d}{dx} [(c_1 + c_2) v] = \mu c_3^0 u \frac{d\eta^*}{dx}, \qquad (3)$$

$$\frac{d}{dx} (c_1 v) = \mu c_3^0 u \frac{d\eta^*}{dx}, \qquad (4)$$

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$$-u \frac{d\eta^*}{dx} = W(T, \eta, c_1), \qquad (5)$$

where

$$\eta = \frac{c_3^0 - c_3}{c_3^0} = \frac{c_4}{c_3^0};$$
(6)

$$W = k \exp\left[-E/RT\right] f(\eta) c_1^n;$$
(7)

$$h_4 = h_3 + \mu h_1; \quad h_i = \int_{T_a}^{T} c p_i \, dT;$$
 (8)

$$c_1 + c_2 = C = P/RT;$$
 (9)

$$\eta^* = \frac{1-s}{2} \eta_{\rm R} + s\eta - \frac{1+s}{2} \eta_0; \tag{10}$$

with s = 1 if the wave travels in the infiltration direction and s = -1 for the opposite one.

We write the boundary conditions for (2)-(5):

$$x \to -\infty$$
 $T = T_0, c_1 = c_1^0, \eta^* = \eta_f^* = \eta_f - \eta_0,$ (11)

$$x \rightarrow +\infty$$
 $T = T_c, c_1 = 0, \eta^* = 0, \frac{dT}{dx} = \frac{d\eta^*}{dx} = 0.$ (12)

The first integrals of (3) and (4) take the form

$$c_2 v = c_2^{\upsilon} v_0, \tag{13}$$

$$c_1 v - c_1^0 v_0 = \mu c_3^0 u (\eta^* - \eta_f^*).$$
(14)

We use (6), (13), and (14) to transform the left side of (2) and integrate the latter once from $-\infty$ to x to get

$$c_{2}^{0}v_{0}h_{2} - suc_{3}^{0}h_{3} + \mu c_{3}^{0}uh_{1}\left(\frac{1-s}{2}\eta_{f} - \frac{1+s}{2}\eta_{0}\right) = \lambda \frac{dT}{dx} - Qc_{3}^{0}u(\eta^{*} - \eta_{f}^{*}).$$
(15)

From (15) with boundary condition (12) we get

$$c_{2}^{0}v_{0}h_{2}^{b} - suc_{3}^{0}h_{3}^{b} + \mu c_{3}^{0}uh_{1}^{b}\left(\frac{1-s}{2}\eta_{f} - \frac{1+s}{2}\eta_{0}\right) = Qc_{3}^{0}u\eta_{f}^{*}; \qquad (16)$$

where the superscript b corresponds to the upper limit in the integral in (8): $T = T_c$. It follows from (5) and (15) that

$$\frac{d\eta^{*}}{dT} = -\left\{ W\left(T, \eta, c_{1}\right) \lambda\left(\eta\right) \right\} \left\{ u \left[c_{2}^{0} v_{0} h_{2} - suc_{3}^{0} h_{3} + \mu c_{3}^{0} u h_{1} \left(\frac{1-s}{2} \eta_{f} - \frac{1+s}{2} \eta_{0} \right) + Q c_{3}^{0} u \left(\eta^{*} - \eta_{f}^{*}\right) \right\}^{-1}$$
(17)

In the approximation used by Zel'dovich and Frank-Kamenetskii [8]

$$c_{2}^{0}v_{0}h_{2} - suc_{3}^{0}h_{3} + \mu c_{3}^{0}uh_{1}\left(\frac{1-s}{2}\eta_{f} - \frac{1+s}{2}\eta_{0}\right) \approx c_{2}^{0}v_{0}h_{2}^{b} - suc_{3}^{0}h_{3}^{b} + \mu c_{3}^{0}uh_{1}^{b}\left(\frac{1-s}{2}\eta_{f} - \frac{1+s}{2}\eta_{0}\right)$$

while (17) and (16) simplify substantially and takes a form known from other papers (in particular [9]):

$$\frac{d\eta^*}{dT} = -\frac{k \exp\left[-E/RT\right] f(\eta) c_i^n \lambda(\eta)}{u^2 Q c_0^2 \eta^*} \,. \tag{18}$$

This approximation enables one to separate the variables in (18) and then to integrate the resulting equation throughout the range of variation to obtain an integral relation between the wave speed and the control parameters T_0 , T_f , η_0 , η_f , which takes the following form for the zeroth-order reaction (n = 0):



Fig. 1. Performance in two-wave infiltration combustion in accordance with extent of reaction on passage of first wave: 1) m = 0, l = 1/2; 2) 0, l = 1; 3) 1, l = 1/2; 4) 1, l = 1; 5) m = -10, l = 0, I) forward waves; II) reverse waves.

Fig. 2. Performance of N-wave forward mode in accordance with final extent of reaction in first wave for given final extents of reaction in the second, third, ..., and N-th waves (abscissas of kink points), m = 1, l = 1: 2) two-wave state; 3) three-wave; 4) four-wave; 5) five-wave.

$$u = \left\{ \left[(k/Qc_3^0) \int_{T_0}^{T_c} \exp\left[-E/RT \right] dT \right] / \int_{0}^{\eta_1^*} \left[\eta^*/f(\eta) \lambda(\eta) \right] d\eta^* \right\}^{1/2}$$
(19)

We use this and specify the forms of $f(\eta)$ and $\lambda(\eta)$ to derive an analytic expression for the velocity ratio u_N/u_1 defining the performance of the multiwave state:

$$\frac{u_{N}}{u_{1}} = \frac{\left\{\int_{0}^{\eta_{f}} [\eta^{*}/f(\eta) \lambda(\eta)] d\eta^{*}\right\}^{1/2}}{\sum_{j=1}^{N} \left\{\int_{0}^{\eta_{f}} \int_{0}^{-\eta_{f}(j-1)} [\eta^{*}/f(\eta) \lambda(\eta)] d\eta^{*}\right\}^{1/2}}.$$
(20)

The following conclusions are drawn. Firstly, $f(\eta)$ and $\lambda(\eta)$ have qualitatively similar effects on this quantity. Further, if the reaction is not retarded by the product $(f(\eta) = 1)$ and the effective thermal conductivity is constant $(\lambda(\eta) = \lambda_0)$, there is no effect from using multiware states: $u_N \equiv u_1$; the situation is different if $f(\eta)$ and $\lambda(\eta)$ vary.

Figure 1 shows calculations from (20) for the two-wave state with a model retardation function $f(\eta) = (1-\eta)^{1/2}$ and the relationship $\lambda(\eta) = \lambda_0(1-m\eta)^*$. Here and subsequently, the final extent of reaction is taken as $\eta_f = 0.95$. This value of η_f has been chosen because it has been shown [10] that there is restricted scope for using the above approximation in incorporating the retardation by the product. An exact (numerical) calculation with $\eta_f = 0.95$ and the maximum retardation considered here has shown that our approximation is permissible.

In discussing the results, we note that the effectiveness of the two-wave state as regards accelerating the process is substantially dependent on the form of $\lambda(\eta)$. If the thermal conductivity falls as the extent of reaction increases, an acceleration can be obtained only in the forward-wave state (curves 1-4), while when the conductivity increases there is

^{*}As the integrals appearing in (20) are tabulated for these cases, detailed working formulas are omitted.



Fig. 3. Dependence of the relative increment in multiwave performance on the passage of wave N in relation to wave number. Symbols as in Fig. 1, $u_N - u_{N-1}/u_2 - u_1$, %.

Fig. 4. Performance of two-wave mixed states in relation to extent of reaction of passage of first wave: I) forward-reverse mode; II) reverse-forward mode. Other symbols as in Fig. 1.

a positive effect dependent on the degree of retardation from the counter-wave state (curve 5). The dependence of the function (u_2/u_1) on the intermediate extent of reaction n_{f1} is of turning-point type in both states.

The maximum propagation speed in the N-wave forward state is provided by minimizing the denominator in (20) with respect to N-1 parameters: n_{f1} , n_{f2} , ..., $n_{f(N-1)}$. We consider this procedure in relation to the three-wave state (Fig. 2). We specify n_{f2} (the values are 0.78, 0.6, 0.93, and 0.85 correspondingly for curves 3, 3', 3", and 3"'), and we optimize the two-wave state with respect to n_{f1} in the range $0 - n_{f2}$. Clearly, the maximum rate is provided with a choice of the upper boundary to the extent of reaction on passage of the second wave $n_{f2} = 0.85$, which is obtained by this minimization. An important point is that the optimum value is $n_{f2} = 0.85$, not 0.78 (the latter corresponds to the maximum speed of the two-wave state with n_f varying from zero to 0.95), as might have been expected at first sight from curves 3' and 3". The optimum three-wave state is realized with the following ranges: 0-0.6 (first wave), 0.6-0.85 (second wave), and 0.85-0.95 (third wave).

The minimization is cumbersome in the general case (N waves), which hinders deriving general relationships for the N-wave state. On the other hand, the general character of the relationships can readily be established by selecting an organization scheme (close to optimal) such that the upper bound to the change in extent of reaction due to wave j, namely nfj, is equal to the extent of reaction providing a maximum speed for the two-wave state involving variation from 0 to nf(j+i) ($j \leq N-1$) (Fig. 2, curves 2-5).

It is clear that as the number of waves increases the effect of using multiwave forward mode increases, and tends to a limiting value for the above falls of $f(\eta)$ and $\lambda(\eta)$ with the above scheme of organization for N \approx 5-6. On the other hand, the relative increment in the performance with each wave passage falls sharply as the number of waves increases, being very slightly dependent on the form of these functions. Figure 3 shows that practical interest attaches to 2-4 wave forward states.

In conclusion we consider multiwave mixed states, where the forward waves alternate with reversed ones and vice versa. Figure 4 shows how the effectiveness in such two-wave states varies with the extent of reaction in the first wave (forward wave for forward-reverse case and reverse wave for reverse-forward case). They show that there is an effect as regards an increase in propagation speed only from the forward-reverse state, with the maximum effect attained in the purely reverse state (one reverse wave).

Also, the calculations show there is an advantage in the one-wave reverse state by comparison with the multiwave forward one, and this is the larger the greater the retardation by the product.

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NOTATION

x, spatial coordinate in the direction of filtration, m; c_1 , c_2 , c_3 , c_4 , molar concentrations of the active component of gas (oxidant), inert component, porous solid material, and reaction product, respectively, mole/m³; h_1 , h_2 , h_3 , h_4 , enthalpies of these components, J/mole; T, current temperature, °K; $\lambda(n)$, thermal conductivity, W/m °K; Q, heat of reaction (per mole of product), J/mole; n, degree of conversion, dimensionless; n_f , finite degree of conversion, ($n_f = 0/1$); μ , stoichiometric coefficient, dimensionless; E, activation energy, J/mole; p, mixture pressure, Pa; R, universal gas constant; v, linear filtration velocity, m/sec; u, linear velocity of reaction wave, m/sec; T_0, c_1° , v_0 , corresponding parameters of cold gas phase; T_c , temperature in the hot part of the layer; c_3° , initial molar concentration of porous material; n, reaction order.

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