REGULARITIES OF THE PROPAGATION OF THE STANDING COUNTERCURRENT WAVE OF AN EXOTHERMAL REACTION IN FORCED FILTRATION OF AN OXIDIZING GAS THROUGH POROUS MATERIAL

O. S. Rabinovich and I. G. Gurevich

The article presents the numerical simulation of the countercurrent wave of an exothermal reaction: the dependences of its characteristics on the "input" parameters of the system.

It was proved in [1] that when an oxidizing gas is blown through a porous medium, it is possible that with the syncurrent wave (in the direction of the flow) there may simultaneously exist a countercurrent wave of the exothermal reaction. However, the results obtained in [1] pertain to the case characterized by constant thermophysical properties of the system, zero order of the reaction, and lack of its inhibition by the forming product. On the other hand, the properties of real systems often do not satisfy these conditions, and this makes it difficult or even impossible to obtain an analytical solution of the corresponding problem of heat and mass exchange. It therefore becomes indispensable to resort to numerical methods of solution.

The system of equations of heat and mass exchange and of the chemical kinetics, describing steady-state wave regimes of the exothermal reaction of the oxidation of a porous material in a system of coordinates moving with the reaction wave, on the assumption that the filtration rate of the gas is much greater than the speed of the waves themselves ($v \gg u$), is analogous to the one used in [2] and has the following form:

$$\frac{d}{dx}[(c_1 h_1 + c_2 h_2)v + (c_3 h_3 + c_4 h_4)u] = \tag{1}$$

$$= \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) + Q c_3^0 u \frac{d\eta}{dx},$$

$$\frac{d}{dx}[(c_1 + c_2)v] = -\mu c_3^0 u \frac{d\eta}{dx}, \tag{2}$$

$$\frac{d}{dx}(c_1 v) = -\mu c_3^0 u \frac{d\eta}{dx}, \tag{3}$$

$$u \frac{d\eta}{dx} = W(T, \eta, c_1), \tag{4}$$

$$\eta = \frac{c_3^0 - c_3}{c_3^0} = \frac{c_4}{c_3^0}, \tag{5}$$

$$W = k \exp[-E/RT] f(\eta) c_1^n, \tag{6}$$

$$f(\eta) = (1 - \eta)^{1/2}, \tag{7}$$

$$c_1 + c_2 = C = P/RT, \tag{8}$$

$$h_4 = h_3 + \mu h_1. \tag{9}$$

The boundary conditions are:

$$x \to -\infty \quad T = T_0, \ \eta = 0, \ c_1 = c_1^0, \tag{10}$$

$$x \to +\infty \quad T = T_\mathrm{r}, \ \eta = \eta_\mathrm{к}, \ c_1 = 0, \ \frac{dT}{dx} = \frac{d\eta}{dx} = 0. \tag{11}$$

In the given statement of the problem it is assumed that the porous material is enclosed in an adiabatic casing that precludes heat losses.

The first integrals of Eqs. (2) and (3) have the form:

$$c_2 v = c_2^0 v_0, \tag{12}$$

$$c_1 v - c_1^0 v_0 = - \mu c_3^0 u \eta. \tag{13}$$

Taking the boundary condition (11) into account, we obtain from (13) the integral ratio

$$u = c_1^0 v_0 / \mu c_3^0 \eta_\text{к}. \tag{14}$$

Moreover, from (8) and (12)-(14) follows the ratio of the local values of oxidizer concentration, temperature, and depth of transformation:

$$c_1 = C^0 \frac{T_0}{T} \left[1 + \frac{\eta_\text{к}}{\eta_\text{к} - \eta} \left(\frac{C^0}{c_1^0} - 1 \right) \right]^{-1}. \tag{15}$$

If we use (5), (12), and (13) for transforming the left-hand side of Eq. (1) and integrated this once from $-\infty$ to x, we obtain

$$c_2^0 h_2 v_0 + \mu c_3^0 u \eta_\text{к} h_1 + c_3^0 h_3 u = \lambda \frac{dT}{dx} + Q c_3^0 u \eta. \tag{16}$$

After substituting the boundary condition (11) into (16), we find yet another integral ratio

$$\eta_\text{к} = \left(\varphi_0 \frac{v_0}{u} + 1 \right) / (q + \xi_0), \tag{17}$$

where

$$\varphi_0 = P h_2^\Gamma / R T_0 c_3^0 h_3^\Gamma, \quad q = Q / h_3^\Gamma, \quad \xi_0 = \mu (h_2^\Gamma - h_1^\Gamma) / h_3^\Gamma. \tag{18}$$

Here and henceforth the index Γ indicates that the values of the corresponding magnitudes are taken in the heated zone ($T = T_\Gamma$, $x = +\infty$).

It follows from (14) and (17) that there is a single-valued correlation between the relative concentration of oxidizer at the inlet to the system and the final depth of transformation of the treated material at the specified temperature in the heated zone (T_Γ):

$$\tilde{c}_1^0 = \frac{c_1^0}{c_1^0 + c_2^0} = \frac{\mu h_2^\Gamma}{\mu (h_2^\Gamma - h_1^\Gamma) + Q - h_3^\Gamma / \eta_\text{к}}. \tag{19}$$

After going over to the independent variable $\theta = T_\Gamma - T$, we obtain the following system of differential equations that are to be integrated:

$$\frac{d\eta}{d\theta} = \frac{W}{uF}, \tag{20}$$

$$\frac{dx}{d\theta} = \frac{1}{F}, \tag{21}$$

where

$$F = - \frac{u c_3^0 h_3^\Gamma}{\lambda} \left[\varphi_0 \frac{v_0}{u} (\tilde{h}_2 - \rho) + (\tilde{h}_3 - \rho) + q (\rho \eta_\text{к} - \eta) \right], \tag{22}$$

$$\tilde{h}_2 = h_2 / h_2^\Gamma, \quad \tilde{h}_3 = h_3 / h_3^\Gamma, \quad \rho = (h_2 - h_1) / (h_2^\Gamma - h_1^\Gamma). \tag{23}$$

Together with the relations (6) and (7) that determine W, and the integrals (12), (14), (15), and (17), Eqs. (20) and (21) were numerically integrated in accordance with the boundary conditions (10) and (11). Some special features of this procedure and the algorithm for the solution were explained in detail in [3].

TABLE 1. Characteristics of the Counterflow Wave in Dependence on the Input Parameters of the System

"Input" parameters				Characteristics of the counterflow wave				
T_0, °K	v_0, m/sec	c_1^0, %	T_Γ, °K	$\eta_{\text{к}}$, b/r	$u \cdot 10^6$, m/sec	$L_p \cdot 10^2$, m	$L_h \cdot 10^2$, m	W/W_0, b/r
300	0,03	3,04	830	0,833	4,28	0,634	1,947	0,243
300	0,03	4,80	830	0,111	50,63	0,389	1,234	0,457

In the numerical calculations, the following values of the kinetic and physical constants were used as an example: $n = 1/2$; $Q = 200$ kJ/mole; $k = 2.1 \cdot 10^8$ $(\text{m}^3/\text{mole})^{1/2} \cdot \text{sec}^{-1}$; $E = 170$ kJ/mole; $\lambda = 0.5 - 0.44\eta$ $(\eta = 0-1)$ W/m·°K; $c_3^0 = 21.0 \cdot 10^3$ mole/m^3; $h_2(T) = 21(T - T_0)$ J/mole; $h_1(T) = 35(T - T_0) + 1 \cdot 10^{-3} (T^2 - T_0^2) + 3.5 \cdot 10^5 \left(\dfrac{1}{T} - \dfrac{1}{T_0} \right)$ J/mole; $h_3(T) = 15(T - T_0) + 2 \cdot 10^{-3}(T^2 - T_0^2) + 1 \cdot 10^6 \left(\dfrac{1}{T} - \dfrac{1}{T_0} \right)$ J/mole.

To study the regularities of the investigated wave regime of the oxidizing reaction, three of its parameters were varied within a wide range of values: $T_0 = 300-550$°K, $T_\Gamma = 800-900$°K, $v_0 = 0.005-0.1$ m/sec.

Going over to the analysis of the obtained results, we want to point out, first of all, that with other conditions (T_0, v_0) being equal, the region in which countercurrent waves exist lies in the range of higher concentrations of oxidizer c_1^0 than for syncurrent waves. Furthermore, it follows from (19) that the process of oxidation in a countercurrent wave regime does not make it possible to ensure an arbitrary depth of transformation of the solid phase (as is the case in the syncurrent wave regime [3]), but that it does so only beginning with

$$\eta_{\text{к}}^* = h_3^\Gamma / (Q - \mu h_1^\Gamma) \tag{24}$$

and higher (up to $\eta_{\text{к}} = 1$); the value of $\eta_{\text{к}}^*$ corresponds to 100% concentration of the oxidizer.

It is worthy of attention that there is no one-to-one correlation between the characteristics of the counterflow wave (T_Γ, $\eta_{\text{к}}$, u, L_p, L_h) and the "input" (independent) parameters of the system (T_0, v_0, c_1^0).

Thus, with the same values of T_0 and v_0 (T_0 being an arbitrary value, while v_0 is higher than some speed v_0^* characteristic of the specified temperature T_0) but two different values of the concentration of the oxidizer c_1^0, two counterflow waves exist with different speeds of propagation, different sizes of the reaction and heating zones, different final depth of transformation of the oxidized material, but with the same temperatures. As an example, Table 1 presents the quantitative characteristics of two such waves.

In accordance with the mentioned peculiarity for the case of the wave of an exothermal reaction examined here, a characteristic feature is the U-shaped aspect of the isothermal ($T_\Gamma = $ const) dependences of the wave characteristics on the filtration speed of the gas: $\eta_{\text{к}}(v_0)$, $u(v_0)$, $c_1^0(v_0)$, $L_p(v_0)$, $L_h(v_0)$, and to the ascending branch of the first of them correspond the descending branches of the next two dependences and the ascending branches of the last two dependences and vice versa (Fig. 1).

It was shown in [4] that the nonuniqueness of the correlation between the wave characteristics and the input characteristics of the system, which we establish and which is far from being obvious, is due to the effect of the inhibition of the counterflow wave by the forming product and of the change of the thermal conductivity of the solid-phase component of the system in proportion to its oxidation on the process of formation and propagation of the counterflow wave of the reaction.

An analysis of the values in Table 1 enables us to suggest a mechanism of the process leading to the regularities shown in Fig. 1. When the concentration of the oxidizer is low, the speed of the reaction is low, and therefore the zone of its localization is relatively broad; this leads to low specific heat liberation (per unit thickness of the layer of material), and consequently to low heat flux and low speed of translation of the reaction wave. As a result, the depth of transformation of the oxidized material is great; this, in turn, additionally reduces the speed of the wave, because of the reduced thermal conductivity and
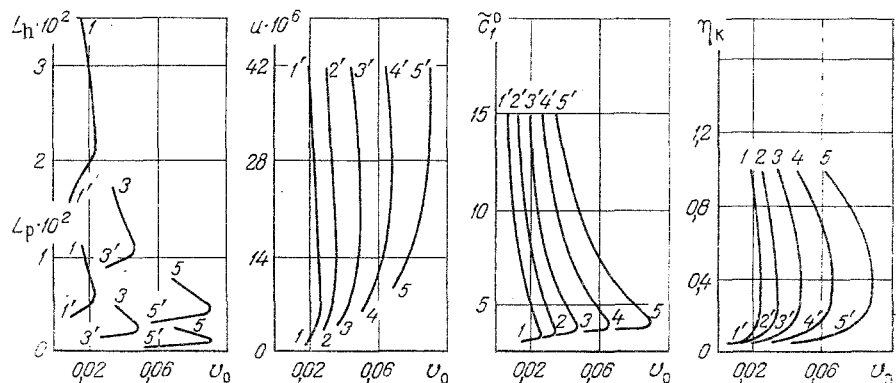
Fig. 1. Dependences of the isothermal characteristics of the counter-flow wave of an exothermal reaction (η_K, b/r; $\tilde{c}_i^o$, %; u, m/sec; L_p, L_h, m) on the filtration speed of the oxidizing gas (v_o, m/sec): 1, 1') T_Γ = 800°K; 2, 2') 825; 3, 3') 850; 4, 4') 875; 5, 5') 900. T_o = 300°K.
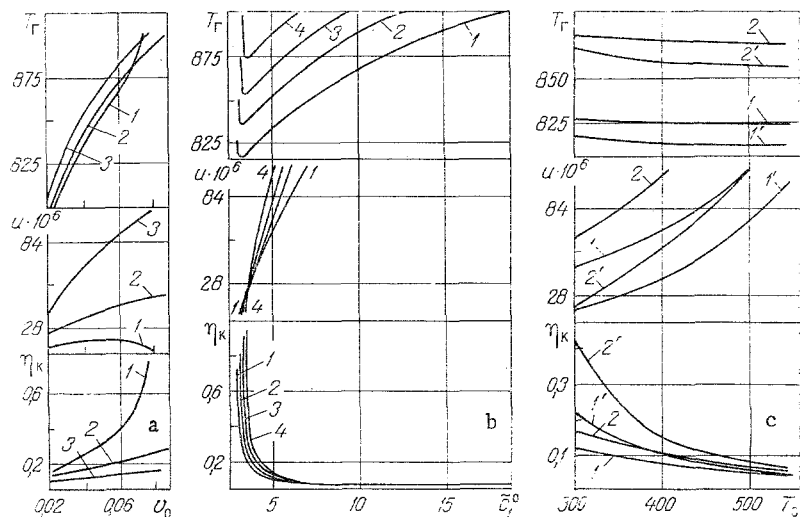

Fig. 2. Dependences of the characteristics of the counterflow wave of an exothermal reaction: a) on the filtration speed of the oxidizing gas [1) $\tilde{c}_i^o$ = 3.5%; 2) 4; 3) 5%], T_o = 300°K; b) on the relative concentration of the oxidizing gas [1) v_o = 0.03 m/sec; 2) 0.04; 3) 0.05; 4) 0.065 m/sec], T_o = 300°K; c) on the gas temperature at the inlet to the layer of test material [1, 1') v_o = 0.03 m/sec; 2, 2') 0.06 m/sec; 1, 2) $\tilde{c}_i^o$ = 4.5%; 1', 2') 3.5%].

increased inhibition of the reaction. Things are different when the concentration of the oxidizer is high: the speed of the reaction is high (in the example under examination, the maximum of its dimensionless value is almost twice as large as this parameter in the case of low concentration of oxidizer), it is localized in a narrower zone, and this means higher specific heat liberation, larger heat flux, and higher speed of propagation of the reaction wave. As a result, the depth of transformation of the material is small. As regards the equality of temperature in the reaction wave T_Γ in both cases (regardless of the substantially larger consumption of oxidizer in one of them), it is ensured by the correspondingly larger heat removal on account of the heating of a larger amount of test material.

Figure 2a-c shows the effect of the input parameters of the system on the principal characteristics of the reaction wave that we examine here.

Increased filtration speed of the gas, with the other two parameters (T_o and c_i^o) constant, leads to increased temperature in the reaction wave, with nonmonotonic nature of the change in its speed of propagation and increased depth (in distinction to the case of the syncurrent wave) of oxidation of the material (Fig. 2a). Yet it must be pointed out that whereas the last of these dependences (η_K = $f(v_o)$) is expressed more weakly with increased

65

concentration of the oxidizer, the second dependence ($u = f(v_0)$) is, conversely, expressed more strongly. Also worthy of attention is the existence of a maximum in the dependence $u = f(v_0)$ and the corresponding change of the curvature of the graphs $T_\Gamma = f(v_0)$. The existence of a maximum in the dependence $u = f(v_0)$ was noted even earlier [1], and it was associated, under the conditions of the problem examined by the authors, with the transition from the regime of incomplete ($\eta_K < 1$) to the regime of complete transformation of the material ($\eta_K = 1$). The same publication also pointed out the simultaneous existence of a maximum in the dependence $T_\Gamma(v_0)$.

Such a "deformation" of the results of the article [1] is a consequence of the inconstancy of the thermophysical characteristics of the system and of the inhibition of the reaction by the product which we took into account.

Increased concentration of oxidizer in the filtered gas mixture, with the other two parameters (T_0 and v_0) being constant, beginning from the minimum concentration corresponding to the beginning of the "region of existence" of the countercurrent wave of the reaction, leads (in distinction to the case of a syncurrent wave) to an abrupt decrease of the depth of oxidation of the test material when the temperature in the reaction wave changes nonmonotonically (with a minimum) and the speed of its propagation increases (Fig. 2b).

And finally, an increase of the gas temperature at the inlet to the system, the other parameters (c_1^0, v_0) being constant in distinction to the case of the current wave, leads to decreased temperature in the wave, to increased speed of its propagation, and to smaller depth of oxidation, yet reduced filtration speed and increased concentration of oxidizer weaken these dependences (Fig. 2c).

Worthy of attention is the practically constant temperature in the reaction wave (the decrease of T_Γ in this example does not exceed 5-10°C) with substantial increase (~200°C) of the inlet temperature of the gas; this is due to the simultaneous increase in heat removal for heating the porous material by increasing the speed of propagation of the wave.

The demonstrated features of interdependence of the parameters of the system and of the wave characteristics according to Figs. 1 and 2a, b are maintained qualitatively for all values of the inlet gas temperature T_0.

NOTATION

x, spatial coordinate in the direction of filtration, m; c_1, c_2, c_3, c_4, molar concentration of the active component of the filtered gas (oxidizer), of its inert component, of the solid porous material, and of the reaction product, respectively, mole/m³; h_1, h_2, h_3, h_4, enthalpies of the above components of the system ($h_i = \int_{T_0}^{T} c_i dT$), J/mole; T, current temperature, °K; $\lambda(\eta)$, thermal conductivity of the solid phase, W/m·°K; Q, thermal effect of the reaction (per mole of product), J/mole; η, depth of transformation of the tested solid phase, b/r; η_K, final depth of transformation ($\eta_K = 0$-1); μ, stoichiometric coefficient of the reaction with respect to the oxidizer, b/r; E) activation energy of the reaction, J/mole; P, pressure of the gas mixture, Pa; R, universal gas constant; v, linear filtration speed, m/sec; u, linear speed of the reaction wave, m/sec; T_0, c_1^0, v_0, the respective parameters of the "cold" gas phase (at the inlet to the layer of test material); T_Γ, temperature in the heated part of the layer of material; c_3^0, initial molar concentration of the porous material; L_p, width of the reaction zone, m; L_h, width of the zone of heating, m.

LITERATURE CITED

1. A. P. Aldushin and B. S. Seplyarskii, "Propagation of a wave of an exothermal reaction in a porous medium when a gas is blown through," Dokl. Akad. Nauk SSSR, 241, No. 1, 72-75 (1978).
2. A. P. Aldushin and B. S. Seplyarskii, "Inversion of the structure of a combustion wave in a porous medium when a gas is blown through," Dokl. Akad. Nauk SSSR, 249, No. 3, 585-589 (1979).
3. O. S. Rabinovich and I. G. Gurevich, "Regularities of the propagation of a syncurrent steady wave of an exothermal reaction in forced filtration of an oxidizing gas through porous material," in: Processes of Heat and Mass Transfer in Bodies with Capillary Pores, Lykov Institute of Heat and Mass Exchange, Academy of Sciences of the Belorussian SSR, Minsk (1982), pp. 21-34.

4. O. S. Rabinovich, "Numerical simulation of waves of an exothermal reaction in forced
    filtration of oxidizer through a porous medium," in: Heat and Mass Transfer: Inves-
    tigations and Development, Lykov Institute of Heat and Mass Exchange, Academy of
    Sciences of the Belorussian SSR, Minsk (1981), pp. 53-57.

EXPERIMENTAL INVESTIGATION OF MASS TRANSFER FROM THE SURFACE OF A SPHERE

UNDER CONDITIONS OF LARGE REYNOLDS NUMBERS AND CAVITATION ON THE SURFACE

G. A. Aksel'rud and S. M. Orel
UDC 66.015.23

The article studies mass transfer from the surface of a sphere when a liquid
flows around it under conditions of Reynolds numbers $10^3 - 5\cdot10^5$, and also
when a cavitation cavern forms behind the sphere.

Article [1] contains the theoretical and experimental investigation of the process of
mass transfer from the surface of a sphere under conditions of small Reynolds numbers. By
proceeding from the concept of the laminar boundary layer, it was possible to calculate
theoretically the mass transport from the frontal part of the surface of a sphere, and
eventually the averaged mass transfer coefficient. It was determined by the equation

$$\mathrm{Nu} = A\,\mathrm{Pr}^{0.33}\,\mathrm{Re}^{0.5}, \quad A = 0.8\text{--}0.95. \tag{1}$$

Equation (1) satisfactorily sheds light on the experimental data in the range Re =
$10^2 - 10^4$ [2].

Later investigations of the hydrodynamics behind a sphere [3] established that there
exists a boundary layer similar to the laminar layer with Re = 60 – 410, thereby confirming
the correctness of Eq. (1). The subsequent investigations [4] revealed that with increasing
Reynolds number the role of the stern part of the sphere in the process of mass transfer as-
sumes greater importance, and when $R > 10^4$, it becomes dominant. It is assumed that the
cause of this is the transition to turbulence of the boundary layer behind the sphere, where-
as on the frontal part the flow in the boundary layer is laminar. This led to the construc-
tion of binomial equations of the type

$$\mathrm{Nu} = \mathrm{Pr}^{0.33}\,(0.51\,\mathrm{Re}^{0.5} + 0.0244\,\mathrm{Re}^{0.78}). \tag{2}$$

This equation is correct for Re = 200 – 200,000 [4]. The present work represents an
attempt at establishing the regularities if mass transfer from the surface of a sphere when
the Reynolds numbers are larger than the investigated range.

The experiments were carried out with an installation whose diagram is shown in Fig. 1.
Water from reservoir 1 is supplied by pump 2 to the glass pipe 5 with 0.1 m diameter in
which were placed spherical particles of 0.025 m diameter made of powdery benzoic acid press-
ed under pressure of 10 MPa. The water in the reservoir was thermostatted. The temperature
was 292±0.5°K.

The installation ensured the possibility of arranging for a lengthy flow around a spher-
ical specimen lasting 60 – 900 sec at speeds of the liquid 0.1–20 m/sec. The mass transfer
coefficient was determined from the loss weight of the specimen before and after the experi-
ment. The flow of liquid through pipe 5 was checked by the induction flow meter 4.

To provide uniform turbulence in the flow around the sphere, screens were placed in
front of the sphere. The first screen 6 with wire diameter $1.5\cdot10^{-3}$ m and mesh size $4\cdot10^{-3}$ ×
$4\cdot10^{-3}$ m was mounted at a distance of 0.44 m from the sphere, and the second screen 7 with
wire diameter $5\cdot10^{-4}$ m and mesh size $8\cdot10^{-3}$ × $8\cdot10^{-3}$ m was mounted at a distance of 0.25 m
from the sphere.

The results of the experiments are presented in Fig. 2. It can be seen from the figure