Journal of Engineering Physics and Thermophysics, Vol. 71, No. 1, 1998

AN APPROXIMATE ANALYTICAL SOLUTION OF THE PROBLEM OF PROPAGATION OF A FILTRATION COMBUSTION WAVE IN A POROUS MEDIUM

S. I. Fut'ko, S. I. Shabunya, and
S. A. Zhdanok

UDC 536.46

Within the one-dimensional single-temperature model, approximate analytical expressions are obtained for determination of the heat wave propagation velocity and the maximum temperature at the combustion front. The present results are compared with the results of the Zel'dovich–Frank-Kamenetskii asymptotic theory.

When a combustible-gas–air mixture filters through an inert porous medium, self-sustaining wave regimes can be observed under certain conditions. To initiate this type of process, it is sufficient to create a narrow high-temperature zone in the porous medium with the aid of an external source (for example, an electric heater) switched on for a time. Subsequently, in the porous medium temperature profiles are formed that propagate at a constant velocity that can be both positive and negative. A review of theoretical and experimental works concerned with this type of combustion is presented in [1]. In particular, theoretical analysis shows that in the absence of heat losses, the maximum flame temperature $T_{\max}$ and the reaction front velocity u_{rw} are related by the simple relation [2]

$$T_{\max} = T_0 + \frac{\Delta T_{\mathrm{ad}}}{1 - \frac{u_{\mathrm{rw}}}{u_{\mathrm{tw}}}}, \tag{1}$$

where ΔT_{ad} is the adiabatic temperature for the given gaseous mixture; u_{rw} is the reaction front wave velocity; u_{tw} is the thermal-wave propagation velocity over the system without reactions.

Equation (1) relates two important parameters of the system, namely, $T_{\max}$ and u_{rw}. It should be noted that inaccuracy in one of them calculated within a certain approximate theory results in a calculation error in the other. While for $T_{\max}$ this is an error in magnitude, for u_{rw} this can even be an error in the direction of the wave propagation.

The goal of the present work is to obtain an approximate analytical solution of the problem of filtration combustion without using an infinitely narrow reaction zone or approximation of the Arrhenius reaction rate, following Frank-Kamenetskii.

We consider the constituting equations that describe combustion waves [2]:

$$(c\rho)_{\mathrm{g}} \frac{\partial T_{\mathrm{g}}}{\partial t} + u_{\mathrm{g}} (c\rho)_{\mathrm{g}} \frac{\partial T_{\mathrm{g}}}{\partial z} = -\alpha (T_{\mathrm{g}} - T_{\mathrm{s}}) + H\rho A K \exp(-U/T_{\mathrm{g}}), \tag{2}$$

$$(c\rho)_{\mathrm{s}} \frac{\partial T_{\mathrm{s}}}{\partial t} = \lambda_{\mathrm{s}} \frac{\partial^2 T_{\mathrm{s}}}{\partial z^2} + \alpha (T_{\mathrm{g}} - T_{\mathrm{s}}), \tag{3}$$

$$\frac{\partial A}{\partial t} + u_{\mathrm{g}} \frac{\partial A}{\partial z} = -AK \exp(-U/T_{\mathrm{g}}), \tag{4}$$

Academic Scientific Complex "A. V. Luikov Heat and Mass Transfer Institute" of the National Academy of Sciences of Belarus," Minsk, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 71, No. 1, pp. 41-45, January-February, 1998. Original article submitted July 2, 1996.

which represent the most important physical processes, such as convective heat transfer in the gas, conductive transfer in the porous skeleton, interphase heat transfer between the gas and the skeleton, and the combustion reaction in the gas phase. In what follows, we consider only regimes that are characterized by high-intensity interphase heat transfer (for example, with a substantial gas flow rate and a small average pore size of the inert medium). Thus, assuming that $\alpha \to \infty$ and $T_g = T_s = T$ and neglecting the thermal inertia of the gas, we can correspondingly simplify Eqs. (2)-(4) to

$$(c\rho)_s \frac{\partial T}{\partial t} + u_g (c\rho)_g \frac{\partial T}{\partial z} = \lambda_s \frac{\partial^2 T}{\partial z^2} + H\rho AK \exp(-U/T)\,, \tag{5}$$

$$\frac{\partial A}{\partial t} + u_g \frac{\partial A}{\partial z} = -AK \exp(-U/T)\,. \tag{6}$$

Having made a changeover to a system of coordinates that moves with the combustion front velocity u_{rw}, $x = z - u_{rw}t$, and assuming that $u_{rw} << u_g$, the system of equations (5), (6) can be rewritten in the following form:

$$T'' - \frac{\tilde{u}}{\lambda} T' = \frac{HG}{\lambda} A'\,, \tag{7}$$

$$\frac{u_0 T'}{T_0} A' = -AK \exp(-U/T)\,, \tag{8}$$

with the definitions

$$\tilde{u} = c_g G \left(1 - \frac{u_{rw}}{u_{tw}}\right), \quad u_{tw} = \frac{u_g (c\rho)_g}{(c\rho)_s}, \quad G = (\rho u)_g = \rho_0 u_0 \tag{9}$$

(the last relation for the gas flow rate G follows from the mass flow continuity equation.)

Next, from physical considerations boundary conditions are chosen for the combustion wave:

$$x = -\infty: \ T' = 0\,, \ T = T_0\,, \ A = 1\,; \tag{10}$$

$$x = +\infty: \ T' = 0\,, \ T = T_{max}\,, \ A = 0\,. \tag{11}$$

Integration of (7) gives

$$T' - \frac{\tilde{u}}{\lambda} T = \frac{HG}{\lambda} A + B\,, \tag{12}$$

where the unknown constant B is determined from boundary conditions (10) and (11), respectively:

$$B = -\frac{\tilde{u}}{\lambda} T_0 - \frac{HG}{\lambda}\,, \quad x = -\infty\,; \tag{13}$$

$$B = -\frac{\tilde{u}}{\lambda} T_{max}\,, \quad x = +\infty\,. \tag{14}$$

Equating (13) and (14), we obtain a balance relation that coincides with (1):

$$(T_{max} - T_0)\,\tilde{u} = HG\,. \tag{15}$$

For a numerical solution of system of equations (7) and (8) with boundary conditions (10) and (11), use is made of some general properties of combustion processes, namely, the fact that because of a strong dependence of the reaction rate on the temperature (relatively high values of the activation energy) and the pronounced exothermic nature of the combustion reaction, chemical conversions can be neglected at temperatures that are much lower than the maximum temperature attained in the flame. Because of this, for numerical calculation, at $A = 1$, $T = T_0$ can be replaced by a certain higher temperature T_-, at which the reaction does not take place (and consequently, the fuel concentration does not change) in the aforementioned sense.

For the procedure of the numerical solution, Eqs. (7) and (8) can be transformed using the dimensionless concentration A (instead of x) as an independent variable and can be reduced to one equation that describes the dependence of the temperature T as a function of the concentration A in the finite range of A: from 1 (the initial mixture) to 0 (the reaction products) with the corresponding temperatures $T = T_-$ and $T = T_{\max}$. In this case

$$T' = T'_A A' . \tag{16}$$

Using the expressions for T' from (12) and A' from (8), we obtain

$$T'_A = -\frac{u_0 T \exp(U/T)}{T_0 KA}\left(\frac{\tilde{u}}{\lambda} T + \frac{HG}{\lambda} A + B\right) . \tag{17}$$

Then, with the aid of (14) and (15), Eq. (17), which describes the relation $T(A)$, can be reduced to the following form:

$$\frac{dT}{dA} = -\frac{u_0 T \exp(U/T)}{\lambda T_0 K}\left(HG + \tilde{u}\frac{T - T_{\max}}{A}\right) . \tag{18}$$

Equation (18) includes the unknown quantity $\tilde{u}$ to be determined in the course of the solution. To do this, the following iteration procedure is organized. An arbitrary value of $\tilde{u}$ is chosen (from a permissible range of values) and the Cauchy problem for (18) with the initial conditions $A = 1$, $T = T_-$ is solved. The calculated quantity $T(0)$ is compared with $T_{\max}$ from balance relation (15). Then, another value of $\tilde{u}$ is chosen, and the cycle is repeated. The iteration is carried out until $T(0)$ coincides with $T_{\max}$ with the required accuracy.

The choice of T_- is not critical since, starting from a certain value, a subsequent decrease in T_- has no effect on the solution. However, the lower T_-, the more accurate (i.e., with a substantially smaller step in A) the calculation procedure near $A = 1$ need be. In the calculations $T_- = 500$ K was used; however, at $T_- = 700$ K the results were the same.

An analysis of calculations for different relations of the parameters shows that the solution of Eq. (18) always has the following properties:

1) the function $\exp(-U/T)$ is almost a linear function of A;

2) a maximum reaction rate (or, according to (7), a maximum of A') is attained at different concentrations A that are somewhat higher than 0.5.

Using property 1), an approximate solution is sought in the form

$$\exp(-U/T) = c_1 (1 - A) , \tag{19}$$

where c_1 is an unknown constant. Determining it from boundary condition (11), we have

$$\exp(-U/T) = \exp(-U/T_{\max})(1 - A) . \tag{20}$$

That there is no identity in expression (20) for $A = 1$ can be explained physically by permissible neglect of the reaction rate at $T = T_0$ (see the explanation of the numerical calculation procedure given above).

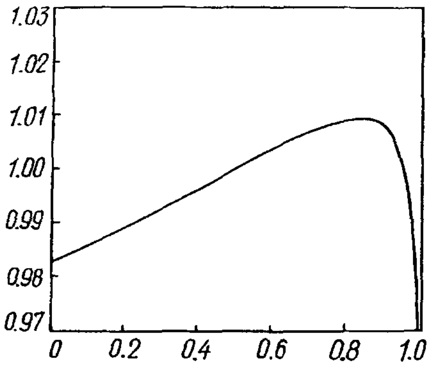

Fig. 1. Plot of the function $F(A)$ normalized to its integral mean value.

Horizontal axis) A; vertical axis) $F(A)/\int_0^1 F(A)dA$

It should be noted that this form of the solution automatically gives property 2). Indeed, we determine the concentration and temperature that correspond to the maximum reaction rate. From the condition of the maximum of the function $A/T \exp(-U/T)$, which is proportional to the reaction rate, we obtain

$$A^* = \frac{1}{2 - T^*/U}, \tag{21}$$

where T^* is the temperature corresponding to the concentration A^*, which is determined from (20) as

$$T^* = \frac{T_{\max}}{2 - \frac{T_{\max}}{U} \ln(1 - A^*)}. \tag{22}$$

Substitution of (22) into (21) gives an expression for A^* from which it is clear that $A^* > 0.5$:

$$A^* = \frac{1}{2 - \frac{T_{\max}}{U}\left(1 - \frac{T_{\max}}{U} \ln(1 - A^*)\right)^{-1}}. \tag{23}$$

Then, for determination of $T_{\max}$, use is made of property 1). To this end, (20) is directly substituted into (18), which gives the following relation:

$$\exp(-U/T) = \exp(-U/T_{\max})(1 - A) F(A), \tag{24}$$

where

$$F(A) = \frac{HG^2 U \exp(U/T_{\max})}{\lambda\rho_0 T_0 K T_{\max}} \left(1 + \frac{T_{\max}}{U}\left(\frac{1}{A(1 - T_0/T_{\max})} - 1\right) \ln(1 - A)\right). \tag{25}$$

Equation (24) is very similar to (20): the only difference consists in the slightly varying function $F(A)$. A plot of this function, normalized on its integral mean value, is shown in Fig. 1. It is a constant quantity to within 2%. The requirement on the value of this constant follows from the requirement of equality of expressions (20) and (24):

$$F(A) = 1. \tag{26}$$

It can be seen from Fig. 1 that to find the equation that determines $T_{\max}$ from (25) and (26), it is natural to take the value of the function $F(A)$, at the point $A = 0.5$ since at this point $F(A)$ coincides with its integral mean value. Thus, the following equation for $T_{\max}$ follows from the condition $F(0.5) = 1$:

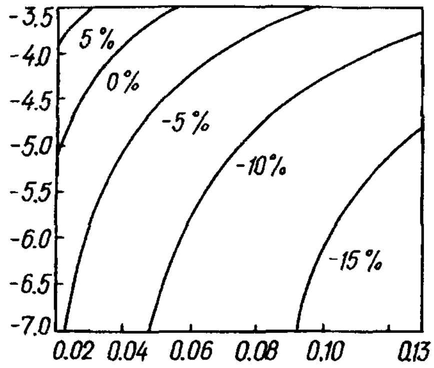

Fig. 2. Difference between T_{max} (%) obtained from (27) and T_{max}^{Zeld} obtained from asymptotic formula (29), following the Zel'dovich–Frank-Kamenetskii's theory, in dimensionless form $(T_{max} - T_{max}^{Zeld})/T_{max}$ for U = 15,640 K, K = 2.6·10^8 sec^{-1}, and λ = 2 W/(m·K). Horizontal axis) dimensionless parameter $\Delta T_{ad}/U$; vertical axis) $\log_{10}((c_g G^2)/(\lambda K \rho_0))$.

$$\exp(-U/T_{max}) = \frac{HG^2U}{\lambda K \rho_0 T_0 T_{max}} \left(1 - \frac{T_{max}^2 \ln 2}{U(T_{max} - T_0)} \left(1 + \frac{T_0}{T_{max}}\right)\right). \tag{27}$$

The value of T_{max} determined from (27) coincides with results of numerical calculations with an error of < 1% for the parameters varying over wide ranges: G = 0.1–20 kg/(m^2·sec) and ΔT_{ad} = 300–2000 K. Use of T_{max} determined from (27) in (20) gives a temperature function $T(A)$ that likewise coincides with the numerical solution with an error of < 1%.

It should also be emphasized that calculations of T_{max} from (27) provide much higher accuracy than the zero-order asymptotic formula (see, for example, [3]). Since problem (7), (8) with boundary conditions (10), (11) is mathematically equivalent to the problem of determination of the normal propagation velocity ω in the Zel'dovich–Frank-Kamenetskii theory of laminar flames, results of this theory [4] can be used directly:

$$\omega^2 \rho_g^2 = \frac{2\lambda K \rho_0 T_0 T_{max}^3 \exp(-U/T)}{c_g U^2 (T_{max} - T_0)^2}. \tag{28}$$

To use this approach in the single-temperature problem of filtration combustion, it is sufficient to substitute $\tilde{u}/c_g$ for $\omega \rho_g$ in Eq. (28). Then, using (15), the following formula can be obtained for determination of T_{max}:

$$\exp(-U/T_{max}) = \frac{H^2G^2U^2}{2\lambda c_g K \rho_0 T_0 T_{max}^3}. \tag{29}$$

Calculations using Eq. (29) show that the accuracy of the calculation of T_{max} is within 20% relative to the numerical results from (18) for a substantial variation in the parameters of the problem: G = 0.1–20 kg/(m^2·sec), ΔT_{ad} = 300–2000 K, and U = 13·10^3–17·10^3 K. Figure 2 shows a comparison of values of T_{max} obtained from (27) with values of it calculated from (29).

In conclusion, it should be noted that Eq. (27), from which, using relation (15), it is possible to find the combustion front propagation velocity, can be used to locate the steady-state combustion zone (the wave velocity u_{rw} = 0) in the quasi-one-dimensional case of a tube with a variable cross section. In this case the position of the reaction zone corresponds to the cross-sectional area S_1 in which the value of the gas flow rate $G = (\rho u)_g$ corresponds to a zero combustion wave propagation velocity for a specified mass flow rate m. Thus, for the case T_{max} = $T_0 + \Delta T_{ad}$, from the continuity equation for the gas mass $m = GS_1$ and Eq. (27) an expression follows that determines the cross-sectional area S_1 in which the combustion reaction zone is localized:

$$S_l = m \left[\frac{\exp\left(U/(T_0 + \Delta T_{ad})\right) HU}{\lambda K \rho_0 T_0 (T_0 + \Delta T_{ad})} \left(1 - \frac{(T_l + \Delta T_{ad}) \ln 2}{U \Delta T_{ad}} (2T_0 + \Delta T_{ad}) \right) \right]^{1/2} . \tag{30}$$

NOTATION

T, temperature; c, specific heat; ρ, density; α, bulk interphase heat transfer coefficient; λ, thermal conductivity; A, dimensionless fuel concentration; U, activation energy; K, preexponential factor; u_0, gas filtration velocity at the ambient temperature T_0.

REFERENCES

1. V. S. Babkin, Pure Appl. Chem., **65**, 335-344 (1993).
2. S. Zhdanok, L. A. Kennedy, and G. Koester, Combust. Flame, **100**, 221-231 (1995).
3. Yu. Sh. Matros, Propagation of Heat Waves in Heterogeneous Media [in Russian], Novosibirsk (1988).
4. D. A. Frank-Kamenetskii, Diffusion and Heat Transfer in Chemical Kinetics [in Russian], Moscow (1987).