Theoretical and Experimental Studies on Laminar Combustion and Detonation Waves

THERMAL THEORY OF A LAMINAR FLAME FRONT NEAR A COLD WALL

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The influence of a cold wall on the shape of a laminar flame front is important for the interpretation of many phenomena connected with the propagation of flames in tubes or between walls, such as quenching, etc.

The present investigation is restricted by the fundamental assumptions of the thermal theory of combustion. Therefore diffusion between the various species is neglected and also the possible effect of a wall on breaking up the chain reactions. Then the effect of the wall in general is twofold: it modifies the flow by friction and the temperature distribution by heat conduction. For most cases the phenomenon is complicated by the fact that the frictional effect extends considerably ahead of the flame. Existence of a secondary motion caused by the flame front is another frequent complicating factor. The authors have tried to find a case where these difficulties do not occur. They consider the case of a flame progressing in a tube of large diameter, filled with an unburned gas mixture; in this case it may be assumed that the one dimensional theory of the laminar flame front can be applied, with the exception of a domain near the wall in which approximately two dimensional flow can be assumed. The problem then is to compute the conditions near the wall. As there is no velocity difference between the unburned gas mixture and the wall at a sufficient distance ahead of the flame, the effect of the wall friction is restricted to the region immediately upstream of the flame front.

The same assumption was used by B. Lewis and G. von Elbe in their treatment of the quenching problem in their book, "Combustion, Flames, and Explosion of Gases" (1). They successfully established useful dimensional correlations between characteristic quantities of the quenching, blow off

and flash back processes. On the other hand, there are also successful attempts to explain quenching on the basis of the pure diffusion theory considering the absorption of activated particles near the wall (2). The present paper cannot bring about a decision between the two different methods of approach; but the authors believe that by introduction of the regular computation methods of Aerothermodynamics they made some progress toward the reduction of the number of arbitrary assumptions, if they can be avoided.

Instead of a laminar progressing wave, the authors consider stationary flow relatively to a flame front at rest. Then one has to assume that the wall is moving with a speed equal to the normal combustion velocity of the gas mixture. The equations for two dimensional steady flow with viscosity, heat conduction and chemical reaction are the following:

(a) Continuity equation

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0. \qquad (1)$$

(b) Momentum equations

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right)$$

$$+ \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) + \frac{1}{3}\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right] \quad (2a)$$

$$+ \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial x}\right) - \frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial y}\right)$$

$$\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial x}\right)$$

$$+ \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y}\right) + \frac{1}{3}\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right] \quad (2b)$$

$$+ \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial x}\right)$$

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(c) Energy equation

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = u \frac{\partial p}{\partial x} + v \frac{\partial p}{\partial y} + \frac{4}{3} \mu \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \frac{3}{4} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2 - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right]$$
$$+ \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) \quad (3)$$

In these equations p, ρ and T denote pressure, density and absolute temperature of the gas mixture relatively, H the total (thermodynamic and chemical) enthalpy per unit mass of the mixture, μ the viscosity coefficient and λ the coefficient of heat conduction; finally u and v are the components of the flow velocity in the x and y directions which are taken parallel and normal to the wall respectively.

For simplicity's sake we neglect the possible changes in the number of molecules during the reaction, so that the gas mixture can be considered as an ideal gas with the average gas constant Rg. Furthermore we do not enter into the details of the chemical reaction, but assume that the chemical enthalpy H_c of the mixture can be written in the form

$$H_c = -q\epsilon$$

where q is the heat release per unit mass of the gas mixture due to the reaction and ϵ is a chemical parameter, the percentage of the end product of the reaction. With these assumptions, the total enthalpy can be written in the following form:

$$H = C_p T - q\epsilon \quad (4)$$

where the sign C_p denotes the specific heat of the mixture at constant pressure taken as constant.

Our computations are carried out for a so-called first order reaction, whose rate follows the Arrhenius law. In this case the chemical parameter is determined by the equation

$$\rho u \frac{\partial \epsilon}{\partial x} + \rho v \frac{\partial \epsilon}{\partial y}$$
$$= K T_0 \rho_0 \frac{1 - \epsilon}{T} exp \left(- \frac{A}{RT} \right), \quad (5)$$

where T_0 and ρ_0 denote the initial absolute temperature and density of the mixture, A is the activation energy and K is a constant of the reaction.

In principle, equations (1) to (5) together with the gas equation and appropriate boundary conditions determine the problem. It is easily seen, however, that due to the complexity of the equations, there is no hope to solve such a problem in the exact way.

In accordance with the usual theory of the laminar flame front, we assume that the pressure changes in the gas are small. In other words we consider deflagration at almost constant pressure. In this case we may neglect in the energy equation the work done by the viscous forces and that due to the small variations of the pressure. Then one obtains the following simplified equation for (3)

$$\rho u C_p \frac{\partial T}{\partial x} + \rho v C_p \frac{\partial T}{\partial y}$$
$$= \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) \quad (6)$$
$$+ \rho q \left(u \frac{\partial \epsilon}{\partial x} + v \frac{\partial \epsilon}{\partial y} \right)$$

The boundary conditions are the following:
At the wall ($y = 0$) and far ahead upstreams ($x = -\infty$):

$$T = T_0, \rho = \rho_0, u = u_0, v = 0, \epsilon = 0$$

where u_0 is the normal combustion velocity.

At infinite distance from the wall ($y = +\infty$) the solution of the system of equations (1), (2a), (2c), (5) and (6) has to approach the solution known from the one dimensional theory of the laminar front.

Hence for $y = +\infty$, $v = 0$ and equation (6) yields:

$$\rho u C_p \frac{dT}{dx} = \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + \rho u q \frac{d\epsilon}{dx}, \quad (6a)$$

where $(\rho u)_{y=\infty} = m$, a constant. Also we want to consider λ as constant[3].

It is useful to introduce a characteristic lenght l of the problem which clearly appears in the energy equation (6a). Such length is given by the formula

$$l = \frac{\lambda}{\rho_0 u_0 C_p} \quad (7)$$

Using this length we introduce non-dimensional variables for the coordinates x and y and also a

[3] Such a solution has been given by the authors in their paper *The Thermal Theory of Constant Pressure Deflagration* (Biezeno Anniversary Volume, Delft, 1953). The solution given in that paper is used for the numerical computations in the present paper.

non-dimensional variable for the temperature by means of the following relations:

$$x = l\xi, \qquad y = l\eta, \qquad T = T_f\theta$$

where T_f is the adiabatic final temperature of the gas mixture. We also note that in the case of constant pressure deflagration the heat release q is equal to

$$q = C_p(T_f - T_0) = C_p T_f(1 - \theta_0)$$

In our paper quoted above, in order to avoid a known difficulty to satisfy the boundary condition at the so-called cold boundary, we assume the existence of a definite ignition temperature. The same assumption is used in this paper. Then there are two domains. The first one in which the temperature is inferior to the ignition temperature T_i (the corresponding value of θ is denoted by θ_i) and the reaction rate is assumed to be zero. In this domain the problem is reduced to one of pure heat conduction and convection. The second domain in which the chemical reaction has to be taken into account is characterized by the condition $T > T_i$.

First let us consider the case that the characteristic length which determines the width of the so-called heating zone is very small, and the rate of reaction is sufficiently large so that the width in which the burning takes place can be also considered as infinitely small. In this limiting case we may assume an infinitely thin laminar flame front, coinciding with the line $x = 0$, which reaches to the wall. Then we have to assume that the temperature is equal to the initial temperature everywhere for $x < 0$ and it jumps at the line $x = 0$ to the value T_f, i.e. the adiabatic combustion temperature.

The problem is now to determine the temperature distribution behind the front, so that the temperature at the wall keeps its value $T = T_0$.

This problem has the character of the boundary layer problems occurring in Fluid Mechanics. One can find a simple solution under the assumptions that the mass flow between parallel lines $y = $ const does not vary with x, and that the heat conduction in the y direction is large in comparison to the heat conduction in the x direction. For this case the continuity equation is satisfied by $v = 0$, $\rho u = m = $ const. and the energy equation takes the simple form

$$mC_p \frac{\partial T}{\partial x} = \lambda \frac{\partial^2 T}{\partial y^2}, \qquad (8)$$

or

$$\frac{\partial \theta}{\partial \xi} = \frac{\partial^2 \theta}{\partial \eta^2}. \qquad (8a)$$

The solution of this equation satisfying the boundary conditions is given by

$$\theta = \theta_0 + (1 - \theta_0)\frac{2}{\sqrt{\pi}} \int_0^{\eta/(2\sqrt{\xi})} e^{-z^2} dz. \qquad (9)$$

The corresponding isotherms are the parabolas shown in figure 1. We will assume that this solution is valid at distances from $x = 0 \quad y = 0$, large in comparison with l. Then the problem is to study
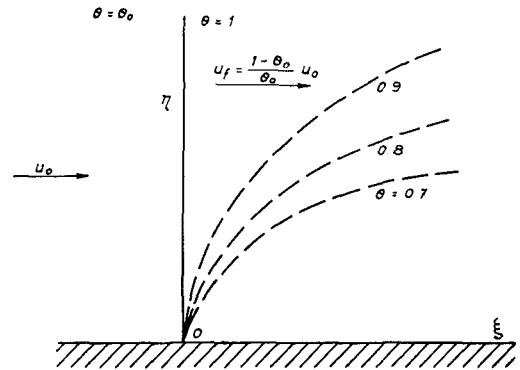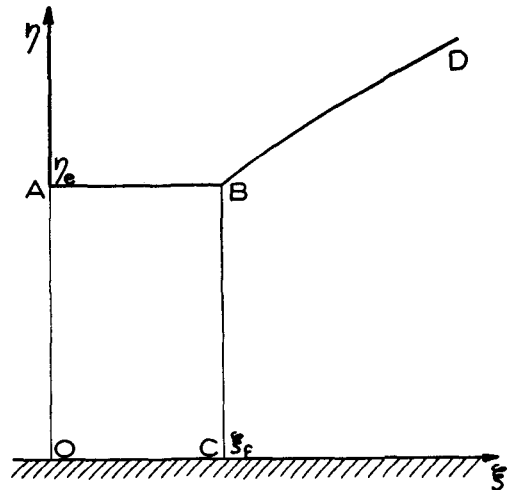

FIG. 1

FIG. 2

what happens in a domain comparable with the characteristic length, i.e. the distortion of the flame front near the wall.

In this paper the authors restrict the computations to the domain $x > 0$ and determine by numerical calculations a temperature distribution satisfying the following conditions shown schematically in figure 2.

(a) the nondimensional temperature θ on $\xi = 0$

and $\eta > \eta_e$ is equal to θ_i, i.e. the ignition temperature of the gas mixture.

(b) on the line AB and for $0 < \xi < \xi_f$, $\eta > \eta_e$ the temperature is determined by the solution of the one dimensional problem. The final temperature theoretically would be reached only at infinite distance. However, the point B, i.e. the values of ξ_f and η_e, were chosen in such a way that at B the deviation from the final temperature as computed from the one dimensional theory is smaller than $\frac{1}{2}$ per cent.

At the same time the parabola BD corresponds to the isotherm $\theta = .995$ according to the approximate theory indicated above (fig. 1).
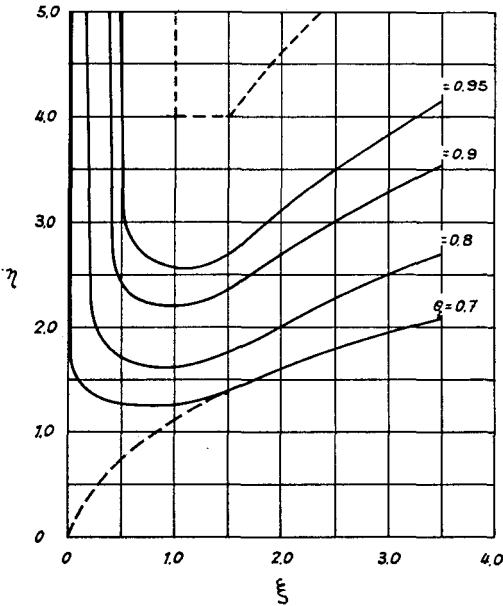

FIG. 3

(c) It is assumed that for $\xi > \xi_f$ the latter theory gives a proper approximation.

Then a solution was computed numerically for the rectangular domain OABC, in such a way that the temperature at CB is equal to the temperature distribution determined from the approximate theory, and along AB is determined by the one dimensional theory. In this computation, heat conduction in both directions was taken into account. Concerning the heat convection, the assumption of constant mass flow was used. In fact it is true that the mass flow has its initial value m immediately at the wall and also outside of the boundary layer. The assumption of constant mass flow also appears justified at larger distances from the origin. It is the belief of the authors, however, that for a more exact theory this assumption should be dropped and a correction calculated.

Using the nondimensional variables and the assumptions made above, the equations (5) and (6) take the form

$$\frac{\partial \epsilon}{\partial \xi} = \frac{\theta_0 Kl}{u_0} \frac{1 - \epsilon}{\theta} e^{-\theta_a/\theta}, \tag{5a}$$

$$\frac{\partial \theta}{\partial \xi} = \frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2} + (1 - \theta_0) \frac{\partial \epsilon}{\partial \xi} \tag{6b}$$

where θ_a is the non-dimensional activation temperature $\theta_a = A/RT_f$.

Instead of integrating the partial differential equations (5a) and (6b) we apply a method similar to the one introduced by the senior author in the theory of boundary layers (Karman's integral equation), and deduce the following integral relation, expressing the balance of heat conduction, heat convection and heat released between neighboring sections ξ and $\xi + d\xi$:

$$\begin{aligned}
\frac{d^2\alpha}{d\xi^2} &= \left(1 - \frac{2}{\theta_e - \theta_0} \frac{d\theta_e}{d\xi}\right) \frac{d\alpha}{d\xi} \\
&+ \left(\frac{d\theta_e}{d\xi} - \frac{d^2\theta_e}{d\xi^2}\right) \frac{\alpha}{\theta_e - \theta_0} \\
&+ \frac{1}{\eta_e} \frac{1}{\theta_e - \theta_0} \left(\frac{\partial\theta}{\partial\eta}\right)_{\eta=0} \\
&- \frac{1}{\eta_e} \frac{1 - \theta_0}{\theta_e - \theta_0} \int_{\eta_i}^{\eta_e} \frac{\partial\epsilon}{\partial\xi} \, d\eta
\end{aligned} \tag{10}$$

In that equation α is defined by the formula:

$$\alpha = \frac{1}{\theta_e - \theta_0} \frac{1}{\eta_e} \int_0^{\eta_e} (\theta - \theta_0) \, d\eta \tag{11}$$

θ_e is the non-dimensional temperature given by the one dimensional theory as function of ξ, and η_i is the value of η corresponding to the ignition temperature.

In order to integrate this equation we assume a one parameter family of temperature distributions:

$$\frac{\theta - \theta_0}{\theta_e - \theta_0} = 1 - \left(1 - \frac{\eta}{\eta_e}\right)^{1/(1-\alpha)} \tag{12}$$

The value of the exponent in equation (12) follows from the definition (11) of α.

The values for α and $d\alpha/d\xi$ at $\xi = \xi_f$ are chosen in such a way that continuity is conserved between the two solutions used for $\xi < \xi_f$ and $\xi > \xi_f$ both as far as the values of the total flux of enthalpy and its derivative with respect to ξ are concerned.

The integration of equation (10) was carried out by stepwise numerical calculation. The resulting temperature distribution is indicated in figure 3.

The obtained temperature distribution corresponds to that expected by qualitative considerations. The isotherm corresponding to the ignition temperature ($\theta = \theta_i$) is almost straight until it is rather suddenly deflected into the direction parallel to the wall and finally joins the parabola obtained by the simplified theory. Taken exactly, some burning may yet occur in the range above the isotherm $\theta = \theta_i$ also for $\xi > \xi_f$ but the calculation showed that the amount of unburned gas in this region is so small that the reaction can be assumed practically finished at $\xi = \xi_f$.

One undesirable feature of the solution is the following: if we calculate the amount of heat transferred through the line $x = 0$ in the sheet between $\eta = 0$ and $\eta = \eta_e$ we find that the heat transferred by convection from the left side to the right side is slightly superior to the amount of heat transferred by conduction from right to left. Since we assume that the solution for values of $\eta > \eta_e$ is identical to the solution of the one dimensional problem, in the range $\eta_e < \eta < \infty$ the total amount of heat transferred from left to right equals that transferred from right to left. Thus we obtain a heat balance which does not provide heat energy for the heat transmission from the gas to the wall ahead of the front. This result shows that the assumption of constant mass flow cannot be exactly correct. If one drops, however, this simplifying assumption, it is necessary to take into account the momentum equations and the problem becomes much more complex.

The width of the dead space for the example carried out in the paper is equal to about 1.25 times the characteristic length, provided we define the dead space as the gap between the wall and the isotherm corresponding to the ignition temperature. In practical measurements the width of the gap between the wall and the luminous region is considered as dead space.

Recently Mr. Kaskan[4] carried out interesting experiments on combustion of methane, propane, and ethylene in air. He measured the dead space defined as the distance between the wall and the luminous border of the flame. The values obtained for stoichiometric mixtures compared with the characteristic length used in this paper are given in table 1.

For the computation of the characteristic length, the data on normal combusion velocity given by M. Gerstein, O. Levine, and E. L. Wong were used (3).

Mr. Kaskan also observed that the dead space is in general considerably smaller than it was thought before, i.e. equal only about $\frac{1}{10}$ of the quenching distance instead of $\frac{1}{3}$ to $\frac{1}{2}$ of this quantity.

However, perhaps, the most important conclusion from these recent experiments—at least from the viewpoint of the authors—is the fact that, according to table 1, the ratio between dead space and characteristic length appears to be almost independent of the nature of the gas used. This may indicate that the thermal conduction is the fundamental characteristic which determines the shape of the flame near a wall. This is the basic assumption of the theory developed in this paper.

The absolute value of the width of the dead space computed in the example given in this paper is considerably smaller than that obtained in Kaskan's experiments. A close accordance cannot be expected, since the assumption on the law of the reaction rate used in the calculations

TABLE 1

Gas	δ	l	δ/l
	mm	mm	
Methane	.3	.051	5.9
Propane	.28	.044	6.36
Ethylene	.18	.027	6.66

δ = dead space.

were rather arbitrary. The main reason for the discrepancy, however, may be the following: The solution used for $\xi > \xi_f$ was based on the assumption that the heat conduction in the main flow direction is small in comparison with the heat conduction crosswise. One finds by direct comparison of the respective heat amounts that, in order to satisfy this condition with fair approximation, a value for ξ_f should be chosen several times larger. It is probable that if the numerical computation will be repeated using larger values for ξ_f, the discrepancy will be essentially reduced.

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