# IGNITION OF A REACTING GAS WITH A HEATED SURFACE, IN THE PRESENCE OF CONCENTRATION DIFFUSION

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The Blasius perturbation method [1] is used to study the effect of reagent burnout and diffusion on ignition characteristics.

Let us examine the ignition of a reacting gas by a heated noncatalytic surface which is suddenly brought into contact with the reacting gas filling a space to the right of the surface. The surface temperature $T_0$ remains constant throughout the entire ignition process, and the initial reagent temperature $T_i < T_0$. Assuming that the thermophysical coefficients of the gas are constant and that we have a reaction of the k-th order, we determine the heating time and the quantity of heat transmitted to the gas by the heated surface during the heating time. Mathematically, the problem reduces to the solution of a system of heat-conduction and diffusion equations [2, 3], which may be expressed in dimensionless form:

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial x^2} + c^k \exp\frac{\theta}{1+\beta\theta}, \tag{1}$$

$$\frac{\partial c}{\partial\tau} = \frac{\partial^2 c}{\partial\xi^2} - \gamma c^k \exp\frac{\theta}{1+\beta\theta} \tag{2}$$

with the following boundary and initial conditions:

$$\theta(0, \tau) = 0, \ \theta(\infty, \tau) = \theta(x, 0) = -\theta_H, \ \left.\frac{\partial c}{\partial\xi}\right|_{\xi=0} = 0, \ c(\infty, \tau) = c(\xi, 0) = 1. \tag{3}$$

If the coefficient of thermal conductivity $\lambda = \lambda_0 T/T_0$, and the density $\rho = \rho_0 T_0/T$, by transformation of the dimensional space coordinate

$$r_1 = \int_0^r \frac{\rho}{\rho_0}\, dr, \tag{4}$$

analogous to the transformation from [4], we can make provision for the relationship between the thermophysical coefficients and the temperature, provided that we are dealing with a first-order reaction. In this case, the form of the heat-conduction and diffusion equations, considering the chemical kinetics, does not change in the dimensionless form, provided – as in [5] – that we assume that $\rho = \rho(T)$ and $\lambda = \lambda(T)$ correspond to the temperature distribution $T(r, t_1)$ at some instant of time $t = t_1$.

We introduce the new independent variables

$$\varepsilon = 4\tau, \quad y = \frac{x}{2\sqrt{\tau}}, \quad \eta = \frac{\xi}{2\sqrt{\tau}}. \tag{5}$$

The system of equations (1) and (2) then assumes the form

$$4\varepsilon\frac{\partial\theta}{\partial\varepsilon} - 2y\frac{\partial\theta}{\partial y} = \frac{\partial^2\theta}{\partial y^2} + \varepsilon c^k \exp\frac{\theta}{1+\beta\theta}, \tag{6}$$

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$$4\varepsilon\frac{\partial c}{\partial \varepsilon}-2\eta\frac{\partial c}{\partial \eta}=\frac{\partial^2 c}{\partial \eta^2}-\gamma\varepsilon c^k\exp\frac{\theta}{1+\beta\theta}. \tag{7}$$

To solve the system of equations (6) and (7), we use the Blasius perturbation method [1], assuming that

$$\theta=\sum_{n=0}^{\infty}\varepsilon^n\theta_n, \tag{8}$$

$$c=\sum_{n=0}^{\infty}\varepsilon^n c_n. \tag{9}$$

Here the subscript n denotes the order of the perturbations. Substituting (8) and (9) into (1) and (2), and collecting terms for identical powers of $\varepsilon$, we find an infinite system of linear boundary-value problems for second-order ordinary differential equations:

$$\frac{d^2\theta_0}{dy^2}+2y\frac{d\theta_0}{dy}=0,\quad \theta_0(0)=0,\quad \theta(\infty)=-\theta_H; \tag{10}$$

$$\frac{d^2c_0}{d\eta^2}+2\eta\frac{dc_0}{d\eta}=0,\quad \left.\frac{dc_0}{d\eta}\right|_{\eta=0}=0,\quad c_0(\infty)=1; \tag{11}$$

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$$\frac{d^2\theta_n}{dy^2}+2y\frac{d\theta_n}{dy}-4n\theta_n=-\psi_{n-1},\quad \theta_n(0)=\theta_n(\infty)=0; \tag{12}$$

$$\frac{d^2c_n}{d\eta^2}+2\eta\frac{dc_n}{d\eta}-4nc_n=\gamma\psi_{n-1},\quad \left.\frac{dc_n}{d\eta}\right|_{\eta=0}=0,\quad c_n(\infty)=0. \tag{13}$$

Here $\psi_{n-1}$ is the corresponding coefficient in the expansion of the function $\psi = c^k\exp(\theta/1+\beta\theta)$ in powers of $\varepsilon$. Having solved the boundary-value problems (10) and (11), we find

$$\theta_0=-\theta_H\,\Phi(y),\quad \Phi(y)=\frac{2}{\sqrt{\pi}}\int_0^y\exp(-z^2)\,dz,\quad c_0=1. \tag{14}$$

The general solution for (12) without the right-hand member has the form

$$\theta_n^{(0)}=A_n\varphi_n+B_n i^{2n}\Phi^*(y),\qquad \varphi_n=2^{-n}\exp(-y^2)\frac{d^{2n}}{dy^{2n}}\exp y^2. \tag{15}$$

The function $i^{2n}\Phi^*(y)$ has been tabulated in [6], and the function $\varphi_n$ can be expressed in terms of the Hermite polynomials [7] of even index and imaginary argument, i.e.,

$$\varphi_n=2^{-n}j^{2n}H_{2n}(jy), \tag{16}$$

where j is an imaginary unit.

Knowing the general solution for the uniform equation, we can use the method of variation for arbitrary constants [8] to find the particular solution, corresponding to $\psi_{n-1}$, and summing (15) and this particular solution, we obtain the general solution for the nonuniform equation:

$$\theta_n=A_n\varphi_n(y)+B_n i^{2n}\Phi^*(y)+2^{n-1}\sqrt{\pi}\int_0^y\psi_{n-1}(z)\,[\varphi_n(z)\,i^{2n}\Phi^*(y)-\varphi_n(y)\,i^{2n}\Phi^*(z)]\exp z^2dz. \tag{17}$$

In analogous fashion, we find

$$c_n=C_n\varphi_n(\eta)+D_n i^{2n}\Phi^*(\eta)-2^{n-1}\sqrt{\pi}\,\gamma\int_0^\eta\psi_{n-1}(\zeta)\,[\varphi_n(\zeta)\,i^{2n}\Phi^*(\eta)-\varphi_n(\eta)\,i^{2n}\Phi^*(\zeta)]\exp\zeta^2d\zeta. \tag{18}$$

Substituting (17) and (18) into boundary conditions (12) and (13), we obtain

$$A_n=2^{n-1}\sqrt{\pi}\int_0^\infty\psi_{n-1}(z)\,i^{2n}\Phi^*(z)\exp z^2dz,\quad B_n=-\frac{\varphi_n(0)\,A_n}{i^{2n}\Phi^*(0)}, \tag{19}$$

$$C_n = -2^{n-1}\sqrt{\pi}\gamma \int_0^\infty \psi_{n-1}(\zeta)\, i^{2n}\Phi^*(\zeta) \exp\zeta^2 d\zeta, \quad \zeta = z\sqrt{L}. \tag{20}$$

We are thus able to find a solution for an infinite system of linear equations (10)-(13) in closed form and, consequently, we can find a solution for the boundary-value problem (1)-(3) in the form of series (8) and (9) in powers of $\varepsilon$.

There arises the question as to the convergence of the series (8) and (9). If $\psi$ is a known function of the argument y, we find the exact solution, since series (8) and (9) terminate. In the general case, when $\psi = c^k \exp(\theta/1 + \beta\theta)$, the convergence of series (8) and (9) could not be proved; however, as will be demonstrated below, the characteristics of the ignition of the reagent by a heated surface for a reaction of zeroth order ($\gamma = 0$) is in good agreement with the results of the numerical calculation [9].

Bringing (8) to a form that will satisfy the Zel'dovich condition [10], i.e.,

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=0} = 0, \tag{21}$$

we find the equation for the determination of the heating time, namely,

$$\frac{2\theta_H}{\sqrt{\pi}} = \sum_{n=1}^{\infty} \frac{i^{2n-1}\Phi^*(0)\,\varphi_n(0)}{i^{2n}\Phi^*(0)} A_n\varepsilon^n. \tag{22}$$

Accurate to perturbations of third and higher orders, Eq. (22) will be quadratic and, solving this equation, for $\beta = 0$ we find the heating time in the form

$$\tau_* = \frac{I_1}{64\sqrt{\pi}(I_2 + I_3)}\left(\sqrt{1 + \frac{16\sqrt{\pi}\theta_H(I_2 + I_3)}{I_1^2}} - 1\right). \tag{23}$$

Knowing the heating time, we can easily find the quantity of heat transmitted by the plate:

$$Q_* = -\int_0^{\tau_*} \left.\frac{\partial\theta}{\partial x}\right|_{x=0} d\tau = 2\sqrt{\frac{\tau_*}{\pi}}\left[\theta_H + \frac{8I_1\tau_*}{3} + \frac{256\sqrt{\pi}}{5}(I_2 + I_3)\tau_*^2\right], \tag{24}$$

where

$$I_1 = \sqrt{\pi}\int_0^\infty \exp[\theta_0(y) + y^2]\, i^2\Phi^*(y)\, dy; \tag{25}$$

$$I_2 = \sqrt{\pi}\int_0^\infty \theta_1(y)\, i^4\Phi^*(y) \exp[y^2 + \theta_0(y)]\, dy; \tag{26}$$

$$I_3 = k\sqrt{\pi}\int_0^\infty c_1(\eta)\, i^4\Phi^*(\eta) \exp[\eta^2 + \theta_0(y)]\, d\eta. \tag{27}$$

The basic contribution to the numerical value of the integrals $I_1 - I_3$ is given by the values of the integrands in the vicinity of zero. In this connection, assuming $\exp\theta_0(y) \approx \exp(-2\theta_H y/\sqrt{\pi})$, which is valid in the vicinity of y = 0, for the calculation of the integrals we employ the Laplace method [11]. As a result we find that

$$I_1 = \frac{\pi}{8\theta_H}\left(1 - \frac{2}{\theta_H} + \frac{3\pi}{2\theta_H^2} - \frac{15\pi}{4\theta_H^3}\right), \tag{28}$$

$$I_2 = \frac{9\pi^{3/2}}{512\theta_H(8 + 3\theta_H)^2}\left[1 - \frac{8}{3\theta_H} + \frac{2}{\theta_H^2}\left(\frac{3\pi}{2} - \frac{8}{9}\right)\right], \tag{29}$$

$$I_3 = -\frac{k\gamma\sqrt{L}\pi}{256\theta_H(1.12840\theta_H + 3.0091)}\left[1 - \frac{2\sqrt{L}}{\theta_H} + \frac{3\pi L}{2\theta_H^2} - \frac{15\pi L^{3/2}}{4\theta_H^3}\right]. \tag{30}$$

Simultaneously with Sidonskii, these same integrals were calculated on an electronic digital computer. Comparison of the data from the numerical calculation and the values of $I_1 - I_3$, found analytically, showed that they are in good agreement with each other. In particular, when $\theta_H = 5, 10, 20, 40$ we have $I_{1S}/I_1 = 1.078$, 1.011, 1.003, 1.000, where $I_{1S}$ denotes the values of $I_1$ obtained by Sidonskii.

Using the fact that $\theta_H \gg 1$, we find the heating time for the ignition of a reagent with a heated plate in the absence of complete reagent burnout ($\gamma = 0$)

$$\tau_0 = \frac{(\sqrt{3}-1)\theta_H^2}{\pi}(1 + 2.82\theta_H^{-1}) \approx 0.233\theta_H^2(1 + 2.82\theta_H^{-1}). \tag{31}$$

The quantity of heat transmitted by the plate is equal to

$$Q_0 = 0.383\theta_H^2(1 + 1.41\theta_H^{-1}). \tag{32}$$

If we limit ourselves exclusively to the first two terms in series (8), we find that

$$\tau_0 = \frac{\theta_H^2}{\pi\left(1 - \dfrac{2}{\theta_H} + \dfrac{3\pi}{2\theta_H^2}\right)} \approx \frac{\theta_H^2}{\pi}, \quad \theta_H >> 1, \tag{33}$$

which corresponds to the Enig results [12].

The asymptotic formulas (31) and (32) agree with the results found with the stress method [5] and the results of the direct numerical calculation [9]. Table 1 gives the values of $\tau_0$ from (31) and the values of $\tau_1$ found by Sidonskii on a digital computer according to (23), in addition to the values of $\tau_2$, obtained by direct numerical calculation [9].

On the basis of these data we can thus contend that the first three terms in series (8) provide a good approximation of the true solution for the boundary-value problem (1)-(3) when $0 \le \tau < \tau_*$. This is explained by the fact that the second and third terms in series (8) (perturbations of the first and second order) are small in absolute value in comparison with the first term when $0 \le \tau < \tau_*$, i.e., the perturbation of the temperature profile as a consequence of the heat of reaction all the way to the instant of time $\tau = \tau_*$ is not great. This remark makes valid the designation of this method as the perturbation method.

If $\gamma\theta_H \ll 1$, and $\theta_H \gg 1$, which according to [9] is valid for nondegenerate ignition regimes, the heating time and the quantity of heat transmitted by the surface will be found from (29) and (30) in the form

$$\tau_* = \tau_0\left\{1 + \sqrt{L}k\gamma\theta_H\left[1 + \frac{2}{\theta_H}(2.67 - \sqrt{L})\right]\right\}, \tag{34}$$

$$Q_* = Q_0\left\{1 + \sqrt{L}k\gamma\theta_H\left[1 + \frac{2}{\theta_H}(2.67 - \sqrt{L})\right]\right\}. \tag{35}$$

It follows from these formulas that the quantities $\tau_*$ and $Q_*$ increase as the order of the k-th reaction increases and with an increase in the quantities $\gamma\theta_H$ and L. It follows from the last that if the coefficient of thermal diffusivity $\varkappa$ is greater than the diffusion coefficient D, i.e., if $L > 1$, to ignite a reacting gas we need a longer heating time than in the case in which $L < 1$.

The numerical analysis of (22) and (23) confirms these qualitative conclusions. Table 2 gives the values of $\tau_*$ and $Q_*$ for various values of L and $\theta_H$, $k = 1$, and $\gamma = 0.01$. It follows from these data that $\tau_*$ and $Q_*$ increase weakly with an increase in L and increase very much more rapidly as $\theta_H$ increases.

We note that the values of $\tau_*$ and $Q_*$, calculated with the aid of the asymptotic values of $I_1$, $I_2$, and $I_3$, virtually do not differ from the corresponding values of $\tau_*$ and $Q_*$, derived by Sidonskii from (23) and (24) with the computer.

In conclusion, we note the Blasius perturbation method [1] enables us to solve the problem of igniting a reacting cylinder at the forward critical point with a stream of heated gas [13], and this method is apparently applicable to the solution of problems involving gas-phase and heterogeneous ignition models.

TABLE 1. Dimensionless Heating Time as a Function of the Dimensionless Temperature Head $\theta_H$ when $\gamma = 0$

| $\theta_H$ | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 100 |
|---|---|---|---|---|---|---|---|---|---|
| $\tau_0$ | 9,11 | 29,87 | 62,20 | 106,34 | 162,05 | 229,41 | 308,43 | 399,08 | 2337 |
| $\tau_1$ | 8,59 | 29,31 | 61,71 | 105,76 | 161,49 | 228,87 | 307,80 | 398,59 | 2395 |
| $\tau_2$ | 10 | 30 | 60 | 100 | 150 | 210 | — | — | — |

TABLE 2. Dimensionless Heating Time and Dimensionless Quantity of Heat Transmitted to the Gas by the Heated Surface as Functions of $\theta_H$ and L

| $\theta_H$ | L | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 0,2 | 0,4 | 0,6 | 0,8 | 1,0 | 1,2 | 1,4 | 1,6 | 1,8 |
| Dimensionless heating time | | | | | | | | | |
| 5 | 8,66 | 8,68 | 8,69 | 8,70 | 8,71 | 8,71 | 8,72 | 8,72 | 8,72 |
| 10 | 29,64 | 29,76 | 29,86 | 29,92 | 29,98 | 30,03 | 30,07 | 30,11 | 30,15 |
| 15 | 62,72 | 63,11 | 63,40 | 63,64 | 63,84 | 64,02 | 64,18 | 64,33 | 64,46 |
| 20 | 108,05 | 108,96 | 109,65 | 110,22 | 110,72 | 111,17 | 111,58 | 111,95 | 112,30 |
| Dimensionless quantity of heat | | | | | | | | | |
| 5 | 17,23 | 17,24 | 17,24 | 17,25 | 17,25 | 17,26 | 17,26 | 17,26 | 17,27 |
| 10 | 64,04 | 64,13 | 64,20 | 64,25 | 64,29 | 64,33 | 64,36 | 64,40 | 64,42 |
| 15 | 139,98 | 140,29 | 140,51 | 140,70 | 140,85 | 140,99 | 141,11 | 141,23 | 141,33 |
| 20 | 245,10 | 245,86 | 246,41 | 246,86 | 247,25 | 247,59 | 247,91 | 248,20 | 248,46 |

## NOTATION

$\theta = (T - T_0)E/RT_0^2$ is the dimensionless temperature;
$\beta = RT_0/E$ is a dimensionless parameter;
$\gamma = c_p\rho RT_0^2/qE$ is a dimensionless parameter;
$x = r\sqrt{(qk_0E/\lambda RT_0^2)\exp(-E/RT_0)}$ is the dimensionless coordinate;
r is a dimensional coordinate;
$\xi = xL$ is a dimensionless coordinate;
$L = \chi/D$;
$\chi$ is the coefficient of thermal diffusivity;
$\lambda$ is the coefficient of thermal conductivity;
D is the diffusion coefficient;
$k_0$ is the preexponent;
$c_p$ is the heat capacity;
$\rho$ is the density;
R is the universal gas constant;
E is the activation energy;
c is the relative reagent concentration;
$\tau = (qk_0Et/c_p\rho RT_0^2)\exp(-E/RT_0)$ is the dimensionless time;
t is the time;
T is the absolute temperature;
$T_0$ is the absolute temperature of the heated surface;
$T_i$ is the initial temperature of the reacting gas;
q is the thermal effect of the reaction;
$\lambda_0$ is the coefficient of thermal conductivity when $T = T_0$;
$\rho_0$ is the density of the gas when $T = T_0$.

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