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Asymptotic analysis of bipropellant droplet burning for the reaction $A+B \rightarrow 2C$

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Abstract—The transport phenomena of convection, diffusion and thermal conduction are analysed for a large-activation-energy burning of a spherical bipropellant droplet. The reaction $A+B \rightarrow 2C$ is assumed to occur in the gaseous phase. The reciprocal value of the activation energy is the small parameter. The two lowest-order terms of the mass flow rate, the flame position and the flame structure are obtained as functions of the nonstoichiometry of the droplet composition. © 1997 Elsevier Science Ltd. All rights reserved.

INTRODUCTION

This paper is devoted to consistent analysis of the single droplet burning for more complex chemistry than just $A \rightarrow B$. An interested reader can find the detailed historical survey in the previous paper [1], which treated the reaction of the arbitrary order (of the type $nA \rightarrow B$).

Numerous investigations have been devoted to the theoretical analysis of a single droplet burning. Earlier papers [2, 3] were based on the thin flame model. The theory taking into account the flame structure, the activation energy and the Lewis number $Le = \lambda/\rho c_p D$ was developed in refs. [4, 5]. But these articles treated a one-dimensional plane deflagration in the gas phase.

The burning of a spherical liquid droplet for $A \rightarrow B$ was first examined by Fendell [6]. The same method as in ref. [6] was then used in refs. [7–11] to treat the droplet burning in various circumstances. However, all these papers treated the same, simplest case $A \rightarrow B$. At the same time, investigations of the plane flame were treated, e.g. a more complex reaction $A+B \rightarrow 2C$ [12–16]; but the droplet case was never investigated for this bimolecular type of chemistry for the premixed case.

Interesting papers [21–24] which appeared recently treat either a plane premixed flame front for the bimolecular chemistry or a droplet burning for the diffusional flame (a droplet consisting of propellant and environs of oxidizer). A bipropellant droplet, to our knowledge, was not treated.

In the present paper we treat the case of the irreversible one-step reaction $A+B \rightarrow 2C$ for the burning of a single spherical droplet.

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ANALYSIS

Consider an isolated droplet consisting of the premixture of two species A and B which can react in the gaseous state according to the bimolecular scheme $A+B \rightarrow 2C$.

The burning is supposed stationary and spherically symmetrical and the droplet having constant radius a due to the large liquid/gas densities ratio. Then the equations of mass conservation and of diffusion and thermal conduction can be put as following [17]:

$$4\pi r^2 \rho v = \text{const.} = M \tag{1}$$

$$\rho v \, \mathrm{d}y_i/\mathrm{d}r - r^{-2}(\mathrm{d}/\mathrm{d}r)(r^2 \rho D \, \mathrm{d}y_i/\mathrm{d}r) = -\rho^2 y_A y_B A \exp(-E/\mathrm{R}T), \quad i = A, B \tag{2}$$

$$\rho v \, \mathrm{d}T/\mathrm{d}r - r^{-2}(\mathrm{d}/\mathrm{d}r)[r^2(\lambda/c_p)\mathrm{d}T/\mathrm{d}r] = \rho^2 y_A y_B (Q/c_p) A \exp(-E/\mathrm{R}T). \tag{3}$$

We suppose that the droplet is not B-lean, that is in any case $y_{A\infty} = 0$. If the mass ratio A/B in the droplet is $\delta \leqslant 1$, then it is easy to derive that $y_{B\infty} = (1-\delta)/(1+\delta)$ (molecular weights of the species are considered equal). Introduce the dimensionless variables $m = (\rho v)_a a/\rho_\infty D_\infty$, $z_i = y_i - (r^2/m)\mathrm{d}y_i/\mathrm{d}r$, $\tau = c_p T/Q$, $\varepsilon = QR/Ec_p$, $L = L_v/Q$, and the first Damkoehler number $D_1 = a^2\rho^2 A/\rho_\infty D_\infty$.

From equations (1) and (2) we can obtain the equations for $y_B - y_A$ and for $z_B - z_A$. Solving them with the condition $(4\pi r^2 \rho D \, \mathrm{d}y_i/\mathrm{d}r)_\infty = 0$ (no diffusion flux at infinity) we are led to $y_B - y_A \equiv y_{B\infty} = \text{const.} = k \geqslant 0$. The smaller k, the closer to the droplet composition stoichiometry. Due to $y_B - y_A = \text{const.}$ we can treat only the equations for A (subscript A is omitted below). In exactly the same way as in ref. [1] these

NOMENCLATURE

A	pre-exponential factor
a	droplet radius
c_p	specific heat capacity
D	diffusion coefficient
D_1	first Damkoehler number
E	activation energy
h	coefficient in flame radius expansion
k	$y_B - y_A$
L	evaporation heat
Le	Lewis number
M	mass flow rate
m	dimensionless mass flow rate
$P_{1,2}(q)$	definite integrals
p	$= Le/(k_1 + 2Le\,\tau_\infty^2)$
Q	reaction heat
q	$= p\tau_\infty^2$
R	gas constant
r	radial coordinate
T	temperature
v	velocity
y	mass fraction of the component A
z	dimensionless mass flow fraction of A.

Greek symbols

δ	mass ratio A/B in the droplet
ε	dimensionless activation energy
Λ	eigenvalue
λ	heat conductivity
ρ	density
τ	dimensionless temperature.

Subscripts

a	droplet surface
f	flame
i	$= 1$ for A, $i = 2$ for B
0, 1, 2	expansion order
∞	far from droplet.

equations could be shown to result in the following ones:

$$dy/d\tau = Le(y-z)/(\tau - \tau_\infty + z) \tag{4}$$

$$dz/d\tau = -y(y+k)r^4 Le\, D_1 \exp(-1/\varepsilon\tau)/ m^2(\tau - \tau_\infty + z) \tag{5}$$

$$dr/d\tau = Le\, r^2/m(\tau - \tau_\infty + z) \tag{6}$$

(now $\tau_\infty = \tau_a - L + z_{Aa}$) with the same boundary conditions as in ref. [1] except for $z(r=1) = z_{Aa} = \delta/(1+\delta)$.

As the method of solution (the method of matched asymptotic expansions [18]) is described in ref. [1], we will not discuss the details here, but will concentrate on the determination of the flame radius $r_f = h_0(\varepsilon)\bar{r}_0$, the terms Λ_0 and Λ_1 in the expansion of the eigenvalue Λ of the problem [see equation (8) below], and the necessary condition $D_1(\varepsilon)$ of the validity of thin flame concept.

Introducing in the same way as in ref. [1] the inner (near τ_∞) and the outer (elsewhere) regions and the corresponding expansions, e.g. $\bar{y}(\bar{\tau}) = \Sigma\varepsilon^i \bar{y}_i(\bar{\tau})$ and $\bar{z}(\bar{\tau}) = \Sigma\varepsilon^i \bar{z}_i(\bar{\tau})$, one easily obtains from equations (4)–(6) that $\bar{y}_1(\bar{\tau}) = Le\bar{\tau}$ with $\bar{\tau} = (\tau_\infty - \tau)/\varepsilon$. Hence it is evident that for various orders of magnitude of k in the small parameter ε we have three cases: (a) $k > O(\varepsilon)$; (b) $k = O(\varepsilon)$; (c) $k = o(\varepsilon)$. However, we will show that (b) and (c) can be described simultaneously [see Section (b)].

(a) *Deviation from stoichiometry greater than the order of the small parameter* ε

In this case equation (5) for the inner region can be changed to

$$dz/d\tau = -kyr^4 Le\, D_1 \exp(-1/\varepsilon\tau) m^2(\tau - \tau_\infty + z), \tag{7}$$

as if we have the first order reaction that has been already considered in ref. [1] for $n = 1$. Introducing

$$\Lambda = (D_1 h_0^4 r_0^4/m^2)\exp(-1/\varepsilon\tau_\infty) \tag{8}$$

but not changing the nomenclature of ref. [1] otherwise, we obtain similarly to ref. [1] (taking into account the changed boundary condition for z):

$$\Lambda = (\Lambda_0 + \varepsilon\Lambda_1)/\varepsilon^2; \quad \Lambda_0 = z_{1a}^2/2Le^2\,\tau_\infty^4,$$
$$h_0 = [k\varepsilon^2 D_1 \exp(-1/\varepsilon\tau_\infty)]^{-1/4}, \tag{9}$$
$$kD_1 = 0[\varepsilon^{-2}\exp(1/\varepsilon\tau_\infty)] \quad \text{for } \varepsilon \to 0,$$

$$r_f = h_0\bar{r}_0 = (1/2)\{1 + [1 - 4Le\,\Lambda_0^{1/2} h_0^2 \times \log(L/z_{1a})]^{1/2}\} \tag{10}$$

$$\Lambda_1/2\Lambda_0 = \{3\tau_\infty + [1.344\sqrt{2}h_0/\bar{r}_0 + \tau_\infty^2 (Le - 2.344)]/z_{1a}\}/[1 - (\sqrt{2}h_0/\bar{r}_0\tau_\infty^2)\log(L/z_{1a})],$$

where 1.344 is the numerical value of $P_1(0)$, see equation (13) below.

(b),(c) *Deviation from stoichiometry of the order of* ε *or less*

As we now have $k = O(\varepsilon)$ then let $k = k_1\varepsilon$ so that $k_1 = O(1)$. In this case like in the case of $n = 2$ of ref. [1] we obtain

$$\Lambda = (\Lambda_0 + \varepsilon\Lambda_1)/\varepsilon^3 \quad h_0 = [\varepsilon^3 D_1 \exp(-1/\varepsilon\tau_\infty)]^{-1/4}$$

$$D_1 = \mathrm{O}[\varepsilon^{-3}\exp(1/\varepsilon\tau_\infty)].$$

The equation for the mass flow fraction is

$$\mathrm{d}\bar{z}_0/\mathrm{d}\bar{\tau} = [\Lambda_0 Le^2\,\bar{\tau}(Le^2\,\bar{\tau}+k_1)/\bar{z}_0]\exp(-\bar{\tau}/\tau_\infty^2)$$

with the boundary condition $\bar{z}_0(0) = 0$. The solution of this equation is of the following form:

$$\bar{z}_0^2 = (2Le^3\Lambda_0\tau_\infty^4/p)\{1-[1+(p\bar{\tau}^2+\bar{\tau})/\tau_\infty^2]\exp(-\bar{\tau}/\tau_\infty^2)\}$$

where $p = Le/(k_1+2Le\,\tau_\infty^2)$. Since matching means $\bar{z}_0(\bar{\tau}\rightarrow\infty)\rightarrow z_{\mathrm{Aa}}$, then $\Lambda_0 = pz_{\mathrm{Aa}}^2/2Le^3\,\tau_\infty^4$. Here, as in Section (a),

$$r_{\mathrm{f}} = h_0\bar{r}_0 = (1/2)\{1+[1-4Le\,\Lambda_0^{1/2}\,h_0^2\log(L/z_{\mathrm{Aa}})]^{1/2}\}$$

but Λ_0 is different. As we have, once again, in the next-to-lowest approximation three different cases for different orders of magnitude of k with respect to ε, we put, formally, $k = \varepsilon k_1+\varepsilon^2 k_2$. Then in the final solution we could substitute $k_2 = 0, k_1 \neq 0$ for the case $k = \mathrm{O}(\varepsilon)$; $k_1 = 0, k_2 \neq 0$ for $k = \mathrm{O}(\varepsilon^2)$; and $k_1 = k_2 = 0$ for $k = \mathrm{o}(\varepsilon^2)$.

The substitution of $\bar{z}(\bar{\tau}) = \bar{z}_0(\bar{\tau})+\varepsilon\bar{z}_1(\bar{\tau})$ to the inner region equations gives

$$\mathrm{d}\bar{z}_1/\mathrm{d}\bar{\tau} = \mathrm{d}\bar{z}_0/\mathrm{d}\bar{\tau}[\Lambda_1/\Lambda_0+(\bar{y}_2+k_2)/(Le\,\bar{\tau}+k_1)+\bar{y}_2/Le\,\bar{\tau}+4h_0\bar{r}_1/\bar{r}_0-\bar{\tau}^2/\tau_\infty^3+(\bar{\tau}-\bar{z}_1)/\bar{z}_0].$$

$$\bar{z}_1 = [1/\bar{z}_0(\bar{\tau})]\int_0^{\bar{\tau}}\mathrm{d}x\bar{z}_0(x)\bar{z}_0'(x)[\Lambda_1/\Lambda_0+(\bar{y}_2(x)+k_2)/(Le\,\bar{\tau}+k_1)+\bar{y}_2(x)/Le\,x+4h_0\bar{r}_1(x)/\bar{r}_0-x^2/\tau_\infty^3+x/\bar{z}_0(x)].$$

Here

$$\bar{y}_2(\bar{\tau}) = Le(1-Le)(\tau_\infty^4/z_{\mathrm{Aa}})\int_0^{\bar{\tau}/\tau_\infty^2}\mathrm{d}x x f(q,x)^{-1/2},$$

$$f(q,x) = 1-(1+x+qx^2)\exp(-x),\quad q = p\tau_\infty^2. \tag{11}$$

Again when matching $\bar{z}_1(\bar{\tau}\rightarrow\infty)\rightarrow 0$ and

$$\Lambda_1/2\Lambda_0 = \tau_\infty^2[2Le\,\Lambda_0^{1/2}\,h_0P_1/z_{\mathrm{Aa}}\bar{r}_0+3(1+2q)/\tau_\infty+(Le-1)(qP_2+2)/z_{\mathrm{Aa}}-P_1/z_{\mathrm{Aa}}-qk_2/2Le\,\tau_\infty^4]/[1-2Le\,\Lambda_0^{1/2}\,h_0/(\bar{r}_0z_{\mathrm{Aa}})\log(L/z_{\mathrm{Aa}})]$$

where

$$P_1 = P_1(q) = \int_0^\infty \mathrm{d}x[1-f(q,x)^{1/2}],$$

$$P_2 = P_2(q) = \int_0^\infty \mathrm{d}x x\exp(-x)f(q,x)^{-1/2}. \tag{12}$$

These integrals are known for some values of q [6, 16, 19], e.g. $P_1(0) = 1.344$, $P_1(1/2) = 2.114$, $P_2(0) = 2$.

Table 1.

δ	ε	h_0	M [g s^{-1}] Ref. [20]	M [g s^{-1}] Present results
1.0	0.06	11.10	$1.1\cdot10^{-4}$	$8.0\cdot10^{-5}$
0.8	0.06	20.00	$1.0\cdot10^{-4}$	$4.4\cdot10^{-5}$
0.8	0.10	0.67	$8.0\cdot10^{-4}$	$9.3\cdot10^{-4}$
0.8	0.30	0.04	$8.0\cdot10^{-1}$	$2.4\cdot10^{-1}$

With $k_2 = 0$, $k_1 \neq 0$ we have the result for the case $k = \mathrm{O}(\varepsilon)$; with $k_2 \neq 0$, $k_1 = 0$ (i.e. $q = 1/2$) for $k = \mathrm{O}(\varepsilon^2)$; with $k_1 = k_2 = 0$ (i.e. $k_2 = 0$, $q = 1/2$) for $k = \mathrm{o}(\varepsilon^2)$ which coincides with the case $n = 2$ of ref. [1].

Dimensional mass flux for the large value of the nonstoichiometry parameter is (only the lowest term is adduced for brevity):

$$M^{(0)} = 4\pi r_{\mathrm{f}}^2\,a^2[2[1-\delta^2)Le\,\lambda\rho^2A/c_{\mathrm{p}}]^{1/2}\delta-1\times(\mathrm{R}T_\infty/E)(c_{\mathrm{p}}T_\infty/Q)\exp(-E/2\mathrm{R}T_\infty).$$

where r_{f} (dimensionless flame radius) is determined by equations (9) and (10).

The presented asymptotic solution can be compared with the results of numerical analysis by Williams [20] of the two-reactant droplet burning for the reaction $F+O\rightarrow 2P$. The droplet was assumed to be of 0.2 mm radius. The results of the comparison are presented in Table 1. We would like to note that only the applicability of the thin flame model is investigated in the present paper, whereas such a restriction does not exist in ref. [20]. Hence, the reader should have in mind that the proximity of the presented h_0s to 1 characterizes the validity of the thin flame model.

CONCLUSION

We have analysed the burning of a droplet of bipropellant fuel for a single chemical reaction of the type $A+B\rightarrow 2C$ for various mixture ratios of the droplet composition. The two lowest-order terms of the mass flow have been calculated. The radius of the thin flame has been determined. The expression for the flame structure has been derived.

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