FUEL POCKET BURNING WITH VARIABLE PROPERTIES

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Abstract

Fuel vapor pockets are formed in several situations, such as leaking of fuel tanks, chemical releases in the atmosphere, pulsed plumes and turbulent flames. A numerical and analytical investigation of fuel pocket burning was made, for different cases: a) a distributed source with variable density and variable diffusivity, b) a distributed source with constant density and constant diffusivity and c) a point source of fuel with constant density and constant diffusivity. Simplified numerical and analytical solutions were obtained and used to estimate the burning times and the maximum flame expansion of fuel pockets of paraffin hydrocarbons, alcohols and carbon monoxide burning in air. It was observed that distributed sources with variable density and variable diffusivity present the largest burning times while point sources of fuel present the largest values of flame expansion. Paraffin hydrocarbons have increasing values of burning times, with increasing molecular weights. Ethanol presents a larger burning time and a larger flame expansion than methanol, but presents lower values of burning time and a larger flame expansion than iso-octane.

Keywords: fuel, pocket, diffusion, flame, burning

1. INTRODUCTION

Fuel vapor pockets can be formed in a number of situations, such as leaking of fuel tanks, chemical releases in the atmosphere, pulsed plumes and turbulent flames. The problem of fuel pocket burning has been studied by several researchers and there are several solutions available in the literature, basically assuming constant properties. Spalding (1959) analyzed the burning of a point source of fuel to simulate supercritical burning of droplets. Rosner (1966,1967) extended Spalding's analysis by considering the burning of a distributed source of fuel. Johari and Motevalli (1993) studied inclusions of fuel vapor pockets appearing in pulsed plumes. Fendell et al. (1994) considered the diffusive burning of spherical and semi-spherical fuel gas pockets in spherical vessels. Costa (1998) considered the effects of differential diffusion on unsteady one-dimensional diffusion flames. The burning times, flame expansion and rates of fuel mass consumption of fuel pockets can be strongly affected by exothermicity. Variable density and variable diffusivity effects can cause a significant increase in the rate of fuel consumption, reduction in burning times and larger flame expansion. A simplified numerical model is developed and used to study the effects of variable density, temperature dependent diffusivity, distributed sources and point sources on the evolution of the diffusive burning of fuel pockets. The numerical solution for the burning of fuel pockets with variable properties is compared to the analytical solutions for constant properties for the cases of paraffin hydrocarbons, alcohols and carbon monoxide burning in air.

2. THEORETICAL ANALYSIS

The present theoretical model considers the diffusive burning of a spherical fuel pocket with equal diffusion coefficients, no radiation effects, no convection effects, no thermal diffusion, isobaric flow, and unity Lewis number. The chemical reaction is assumed to occur in a single step with s Kg of oxidizer reacting with 1 Kg of fuel, i.e., $1F + sO \rightarrow (1+s)P$. Consequently, the mass conservation, species conservation and energy conservation equations are given, respectively, by

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial\left(\rho r^2 \mathrm{v}\right)}{\partial r} = 0 \tag{1}$$

$$\rho\left(\frac{\partial Y_i}{\partial t} + \mathrm{v}\frac{\partial Y_i}{\partial r}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho D r^2 \frac{\partial Y_i}{\partial r}\right) + w_i \tag{2}$$

$$\rho\left(\frac{\partial h}{\partial t} + \mathrm{v}\frac{\partial h}{\partial r}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho D r^2 \frac{\partial h}{\partial r}\right) + w_F \Delta H_r \tag{3}$$

where ρ is the total density, v is the flow velocity, t is the time, r is the position coordinate, Y_i is the mass fraction of the species i, D is the diffusion coefficient, h is the total specific enthalpy, w_i is the generation rate of species i, ΔH_r is the heat of reaction. Figure 1 shows a scheme of a burning fuel pocket, with initial diameter $2a$ and initial mass fractions of fuel and oxidizer $Y_{F,0}$ and $Y_{O,0}$, respectively.

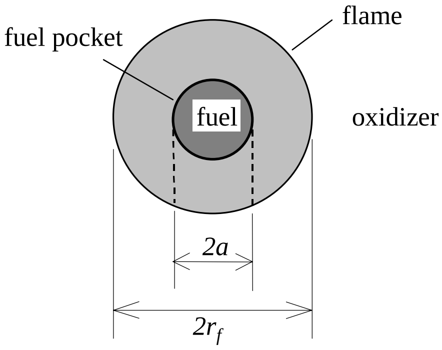

Figure 1. Scheme of a spherical fuel pocket.

In order to eliminate the reaction terms in equations (2) and (3), the following normalized Schvab-Zel'dovich variables β_i ($i=F,O,P,T$) are defined:

$$\beta_i = \frac{1 + \phi\dfrac{Y_F}{Y_{F,0}} - \dfrac{Y_O}{Y_{O,0}}}{1+\phi} = 1 - \frac{\phi}{1+s}\frac{Y_P}{Y_{F,0}} - \frac{Y_O}{Y_{O,0}} = \frac{Y_F}{Y_{F,0}} + \frac{C_P\left(T - T_0\right)}{Y_{F,0}Q} \tag{4}$$

where $\phi = s\,Y_{F,0}/Y_{O,0}$ is defined as being an initial equivalence ratio or an initial F/O ratio of the fuel and oxidizer on the two sides of a diffusion flame, and $Q=-\Delta H_r$ is the heat release. The flame position, assuming fast chemistry, is found by setting $Y_F = Y_0 = 0$ in the above variables, yielding $\beta_i = 1/(1+\phi) = \beta_f$. Table 1 shows values of s, ϕ and β_f for several fuels burning in air and $Y_{F,0} = 1$. Also, the flame temperature T_f is found by setting $Y_F = Y_0 = 0$ in the Shvab-Zel'dovich variable for temperatures in Eq. (4).

After combining equations (2) and (3), the following equation for β_i is obtained:

$$\rho\left(\frac{\partial\beta_i}{\partial t} + v\frac{\partial\beta_i}{\partial r}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho D r^2 \frac{\partial\beta_i}{\partial r}\right) \tag{5}$$

with initial/boundary conditions

$$\beta_i(|r| < a, t = 0) = 1; \qquad \beta_i(|r| > a, t = 0) = 0; \qquad \beta_i(|r| \to \infty, \forall t) = 0 \tag{6}$$

The variables β_i correspond to mixture fraction variables, since they are normalized and Equation (5) does not have a source term. Ignition is assumed to occur instantaneously at all points of the fuel-oxidizer interface. Ignition will probably occur in the stoichiometric locus, as showed by Liñán and Crespo (1976). Assuming a fast consumption of the interpenetrated reactants, the flame evolution after ignition will proceed according to the conventional Burke-Schumann solution (1928), as long as the characteristic reaction time is kept significantly less than the characteristic diffusion time during the burning process.

Table 1. Properties of several fuels burning in air ($Y_{F,0} = 1$)

Fuel	β_f	ϕ	s	D_o (cm^2/s)	c_P (kJ/Kg/K)	T_f (K)	k
CO	0.2484	2.48	5.710	0.214	1.2829	2580	26.253
CH4	0.0544	17.39	4.000	0.226	3.8504	1015	43.294
C3H8	0.0595	15.81	3.636	0.121	3.5736	1080	43.235
nC4H10	0.0603	15.59	3.586	0.097	3.5323	1090	43.139
nC6H14	0.0611	15.37	3.535	0.079	3.4975	1100	42.984
iC8H18	0.0615	15.25	3.508	0.069	3.4669	1100	42.889
CH3OH	0.1330	6.52	1.500	0.161	2.7695	1325	25.387
C2H5OH	0.0993	9.07	2.087	0.118	3.0277	1220	30.530

In order to eliminate the convective terms in the governing equations, a material transformation is utilized by defining two new variables, $\tilde{\tau}$ and $\tilde{\eta}$:

$$\tilde{\tau} = t \quad \text{and} \quad \tilde{\eta} = 3\int_0^r \left(\frac{r}{a}\right)^2 \frac{\rho}{\rho_0}\, dr\,. \tag{7}$$

At t=0, when $\rho = \rho_0$, this choice of variables yields $\tilde{\eta} = a$ for $r = a$, and $\tilde{\eta} = 0$ for $r = 0$. Introducing the two new variables into Equations (1) and (5), it follows that

$$\frac{\partial\rho}{\partial\tilde{t}} + 3\frac{\rho^2}{\rho_0}\frac{\partial}{\partial\tilde{\eta}}\left(\tilde{v}\left(\frac{r}{a}\right)^2\right) = 0 \tag{8}$$

$$\frac{\partial \beta_i}{\partial \tilde{t}} = 9 D_0 \frac{\partial}{\partial \tilde{\eta}}\left(\left(\frac{r}{a}\right)^2 \frac{\partial \beta_i}{\partial \tilde{\eta}}\right) \tag{9}$$

In Eq. (9), it was assumed that $\rho^2 D$ = constant, since $D \sim T^c$, with $1.75 < c < 2.0$, and $\rho \sim T^{-1}$, for an isobaric process. D_0 is the diffusion coefficient value at the initial temperature T_0 = 300 K and $\tilde{v}$ is the flow velocity in the transformed space. Table 1 shows values of D_0 for several fuels. In terms of the non-dimensional variables $\bar{\eta} = \tilde{\eta}/a$, $\eta = r/a$, $\bar{v} = \tilde{v}a/D_0$ and $\bar{\tau} = \tilde{\tau} D_0/a^2$, the conservation equations (8) and (9) become

$$\frac{\partial}{\partial \bar{\tau}}\left(\frac{\rho_0}{\rho}\right) = 3 \frac{\partial}{\partial \bar{\eta}}\left(\bar{v}\eta^2\right) \tag{10}$$

$$\frac{\partial \beta_i}{\partial \bar{\tau}} = 9 \frac{\partial}{\partial \bar{\eta}}\left(\eta^4 \frac{\partial \beta_i}{\partial \bar{\eta}}\right) \tag{11}$$

where the non-dimensional position coordinate in the physical space, η, is related to the non-dimensional position coordinate in the transformed space, $\bar{\eta}$, by

$$\eta = \left(\int_0^{\bar{\eta}} \frac{T}{T_0} d\bar{\eta}\right)^{1/3} \tag{12}$$

for the case of diluted reactants or for reactants and products with equal molecular weights. The temperature ratio is obtained from the definitions of the Schvab-Zel'dovich variables:

$$\frac{T}{T_0} = 1 + \frac{k}{\phi}\left(1 - \beta_i\right) \qquad \left|\bar{\eta}\right| < \left|\bar{\eta}_f\right| \tag{13}$$

$$\frac{T}{T_0} = 1 + k\beta_i \qquad \left|\bar{\eta}\right| > \left|\bar{\eta}_f\right| \tag{14}$$

where $\left|\bar{\eta}_f\right|$ is the absolute value of the flame position in the transformed space and $k = QY_{F,0}/C_P/T_0$. The flame temperature is given by $T_f = T_0\left(1 + k\beta_f\right)$. Values of k, c_p and T_f for several fuels are shown in table 1. The specific heat c_p was calculated at the average temperature $T_{av} = (T_0 + 2T_f)/3$.

Substituting the temperature ratio expressions, given by equations (13,14) into the evolution equation for the mixture fraction, Eq. (11), it follows that

$$\frac{\partial \beta_i}{\partial \bar{\tau}} = \frac{\partial}{\partial \bar{\eta}}\left(\alpha\left(\bar{\eta}, \bar{\tau}, \beta_i\right) \frac{\partial \beta_i}{\partial \bar{\eta}}\right) \tag{15}$$

where

$$\alpha(\eta, \tau, \beta_i) = 9\left[\left(1 + \frac{k}{\phi}\right)\bar{\eta} - \frac{k}{\phi}\int_0^{\bar{\eta}} \beta_i d\bar{\eta}\right]^{\frac{4}{3}} \qquad \left|\bar{\eta}\right| < \left|\bar{\eta}_f\right| \tag{16}$$

$$\alpha(\eta,\tau,\beta_i) = 9\left[\eta_f^3 + \overline{\eta} - \overline{\eta}_f + k\int_{\overline{\eta}_f}^{\overline{\eta}} \beta_i d\overline{\eta}\right]^{\frac{4}{3}} \quad |\overline{\eta}| > |\overline{\eta}_f| \tag{17}$$

with initial and boundary conditions

$$\beta_i\left(|\overline{\eta}| < 1, \overline{\tau} = 0\right) = 1;\ \beta_i\left(|\overline{\eta}| > 1, \overline{\tau} = 0\right) = 0;\ \beta_i\left(|\overline{\eta}| > 1, \overline{\tau} = 0\right) = 0;\ \beta_i\left(|\overline{\eta}| \to \infty, \overline{\tau} > 0\right) = 0 \tag{18}$$

The flame position in the transformed space, $\overline{\eta}_f$, is located where $\beta_i = 1/(1+\phi) = \beta_f$. Equation (10) can be integrated with respect to the position coordinate, for a fixed time, yielding an expression for the induced flow velocity, $\overline{\mathrm{v}}$:

$$\overline{\mathrm{v}} = \frac{1}{3\eta^2}\int_0^{\overline{\eta}} \frac{\partial}{\partial\overline{\tau}}\left(\frac{\rho_0}{\rho}\right) d\overline{\eta} \tag{19}$$

A similar expression was obtained by Ramos (1987) for the burning of premixed flames. The flame position in the variable density problem is obtained from Eq. (12):

$$\eta_f = \left(\int_0^{\overline{\eta}_f} \frac{\rho_0}{\rho} d\overline{\eta}\right)^{1/3} \cong \left(\int_0^{\overline{\eta}_f} \frac{T}{T_0} d\overline{\eta}\right)^{1/3} = \left[\overline{\eta}_f + \frac{k}{\phi}\int_0^{\overline{\eta}_f} (1-\beta_i) d\overline{\eta}\right]^{1/3} \tag{20}$$

The mass rate of fuel consumption per unit flame area for the variable density diffusive burning, $\dot{m}_{FVD}$, is given by the expression

$$\dot{m}_{FVD} = \rho D \left.\frac{\partial Y_F}{\partial r}\right|_{r_f} = 3\frac{\rho_0 D_0 Y_{F,0}}{a}\frac{1+\phi}{\phi}\eta_f^2 \left|\frac{\partial\beta_i}{\partial\overline{\eta}}\right|_{\overline{\eta}=\overline{\eta}_f} \tag{21}$$

and, consequently, the ratio of the fuel mass consumption rates per unity flame area for variable density, $\dot{m}_{FVD}$, and constant density, $\dot{m}_{FCD}$, burning is given by

$$\frac{\dot{m}_{FVD}}{\dot{m}_{FCD}} = 3\eta_f^2\left(\left|\frac{\partial\beta_i}{\partial\overline{\eta}}\right|_{\overline{\eta}=\overline{\eta}_f} \Bigg/ \left|\frac{\partial\Phi}{\partial\eta}\right|_{\eta=\eta_f}\right) \tag{22}$$

where Φ is the solution for a constant density fuel pocket.

3. CONSTANT DENSITY FUEL POCKET

The governing equations in terms of mixture fraction, for the burning of a distributed source or spherical fuel pocket with constant density and constant diffusivity is given by

$$\frac{\partial\beta_i}{\partial\tau} = \frac{1}{\eta^2}\frac{\partial}{\partial\eta}\left(\eta^2\frac{\partial\beta_i}{\partial\eta}\right) \tag{23}$$

where $\tau = tD_0/a^2$ and $\eta = r/a$ are the non-dimensional time and position coordinates in the physical space. The initial and boundary conditions are normalized. Solution for a similar initial-value problem was presented by Carslaw and Jaeger (1959), and by Rosner (1966,1967) for a distributed source of fuel. It can be written as $\beta_i = \Phi(\eta, \tau)$ with the function Φ given by

$$\Phi = \Phi_0 - \left(\sqrt{\tau/\pi}/2\eta\right)\left[\exp\left(-(1-\eta)^2/4\tau\right) - \exp\left(-(1+\eta)^2/4\tau\right)\right] \tag{24}$$

where $\Phi_0 = \left(erf\,(1-\eta)/\sqrt{4\tau} + erf\,(1+\eta)/\sqrt{4\tau}\right)/2$.

The flame position η_f can be found by setting $Y_F = Y_0 = 0$ in the reactant Shvab-Zel'dovich variables defined in Eq. (4), yielding

$$\Phi(\eta_f, \tau) = 1/(1+\phi) = \beta_f \tag{25}$$

The burning times τ_b are determined by taking the limit $\eta_f \to 0$ in the above expression, resulting in $\Phi(0, \tau_b) = \beta_f$. For a given initial composition, determined by β_f, the value of τ_b is a constant.

Temperature and mass fraction profiles can be found by using the definitions given by Eq. (4), and setting $Y_F = 0$ in the oxidizer side and $Y_O = 0$ in the fuel side, once the flame position is known. The rate of fuel mass consumption per unit flame area is given by

$$\dot{m}_F = \rho D \left.\frac{\partial Y_F}{\partial r}\right|_{r_f} = \frac{\rho_0 D_0 Y_{F,0}}{a}\frac{1+\phi}{\phi}\left|\frac{\partial \Phi}{\partial \eta}\right|_{\eta=\eta_f} \tag{26}$$

and the percentage of residual fuel mass inside the flame zone is obtained from

$$\frac{m_F}{m_{F,0}} = 3\int_0^{\eta_f}\frac{Y_F}{Y_{F,0}}\eta^2 d\eta = 3\frac{1+\phi}{\phi}\int_0^{\eta_f}\left(\Phi - \beta_f\right)\eta^2 d\eta \tag{27}$$

3. POINT SOURCE OF FUEL

Spalding (1959) obtained a solution for the diffusive burning of a point source of fuel with constant density. The flame position and burning time are given, respectively, by

$$\frac{r_f}{4Dt} = \ln\left(\frac{M_f}{\rho\beta_f(4\pi Dt)^{3/2}}\right) \tag{28}$$

and

$$t_b = \frac{1}{4\pi D}\left(\frac{M_f}{\rho\beta_f}\right)^{2/3} \tag{29}$$

where M_f is the mass of fuel injected into the system at time $t = 0$. The maximum flame position is obtained from

$$r_{\max} = \frac{3}{2\pi e}\left(\frac{M_f}{\rho\beta}\right)^{2/3} \qquad (30)$$

4. RESULTS

A comparison of the models presented were made for paraffin hydrocarbons, alcohols and carbon monoxide burning in air. Equation (25) was used to obtain burning times and maximum flame positions for the constant density cases, assuming $D = D_0$. Equations (30) and (31) where used for the cases assuming a point source of fuel, with $D = D_0$. Equations (15) through (18) where numerically integrated, using an explicit finite difference scheme with variable time step, total grid sizes of 400, 500 and 600, with 40, 50 and 60 grid points for the fuel region.

Figure 2 shows the burning times of fuel pockets with variable density (VD), constant density (CD) and a point source of fuel (PS) versus non-dimensional time for unsteady one-dimensional diffusion flames with variable density and fast chemistry, for paraffinic fuels, methanol, ethanol and carbon monoxide reacting with air. Fig. 3 shows the maximum flame expansion for the same fuels.

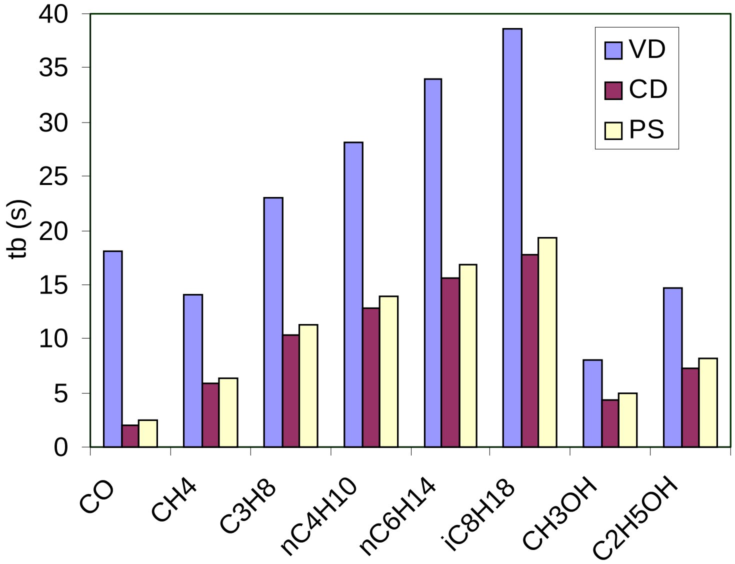

Figure 2. Burning times of fuel pockets with variable density (VD), constant density (CD) and a point source of fuel (PS).

5. CONCLUSIONS

Simplified analytical and numerical solutions were utilized to investigate the effects of variable density, variable diffusivity, distributed sources and point sources on the diffusive burning of fuel pockets of paraffin hydrocarbons, alcohols and carbon monoxide burning in air. The results obtained show a strong influence of the variable density and of the distributed source effects on the diffusive burning of fuel pockets.

It was observed that distributed sources with variable density and variable diffusivity present the largest burning times while point sources of fuel with constant density and constant diffusivity present the largest values of flame expansion.

Paraffin hydrocarbons have increasing values of burning times, with increasing molecular weights. Ethanol presents a larger burning time and a larger flame expansion than methanol, but presents lower values of burning time and larger flame expansion than iso-octane. Carbon monoxide is most significantly influenced by variable density and variable diffusivity effects on burning times, due to its low specific heat and higher flame temperature. Exothermicity induces a flow field that presents a rapid decay after ignition and increases the maximum flame expansion compared to a distributed source of fuel with constant density. Flame expansion increases the time required to the reactants diffuse to the flame zone, decreasing fuel consumption. Other effects, such as lower densities due to exothermicity, flame area stretching, stretching of reactant profiles and diffusivity variations strongly affect fuel mass consumption.

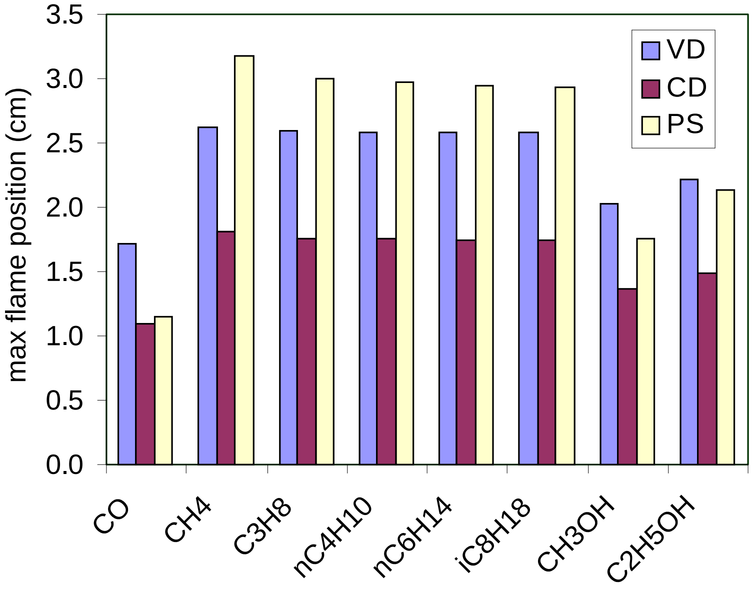

Figure 3. Maximum flame positions of fuel pockets with variable density (VD), constant density (CD) and a point source of fuel (PS).

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