A THEORETICAL INVESTIGATION ON THE KINETIC AND RADIATIVE EXTINCTION OF SPHERICAL DIFFUSION FLAMES IN MICROGRAVITY

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ABSTRACT

Thrust and fire safety are among NASA's major concerns in the fulfillment of its mission on Mars Exploration, especially the missions that planned to bring astronauts to and back from the Red Planet. Responding to these concerns, the research studied the burning characteristics and extinction of diffusion flames in space, which are different from those on Earth due to the lack of gravity. Because microgravity combustion experiments require special facilities available only in NASA and are very costly, the investigation is theoretical that includes analytical and computational contents. In the analytical study, a mathematical model was formulated to identify the flame location, flame temperature, and extinction condition. The computational study was performed using an existing flame code that incorporated detailed chemistry and transport properties. The analytical study focuses on the steady burning while the computational study on the transient behavior of flames. Spherical flames stabilized by a porous burner were used in this research. It was observed that Lewis number of fuel in the ambient has a profound impact on the kinetic extinction state. From the numerical analysis, it was observed flames with a higher flow rate extinguish quicker due to the radiative heat loss .

INTRODUCTION

In recent years, the primary interest of NASA is focused on the exploration of Mars, which includes launch of spacecraft carrying astronauts to and back from Mars. Thrust and fire safety are among NASA's major concerns to fulfill this most challenging mission. In a space travel, as on earth, thrust is provided by the reaction between the fuel and the oxidizer. To provide thrust, the flame is required to burn as strong as possible and extinction should be avoided. During the trip, fire outbreak can also occur from various ignition sources such as radiation from the Sun. Such accidents need to be prevented because external assistance is unavailable when a fire burst out and the result could be disastrous. If a fire accident happens, the flame needs to be extinguished as fast as possible to minimize the damage. In most of practical combustion systems, including those used to provide thrust in space travels and related to undesired fire incidents, the flames are non-premixed. The fuel and oxidizer are supplied from separated sources and transported through convection and molecular diffusion to the reaction region within which they meet and react to produce products and heat. The flame is also known as diffusion flame.

Realizing the needs, the research studied the burning characteristics and extinction conditions of diffusion flames stabilized by a spherical porous burner in microgravity. By employing this type of burner, different factors that affect the flame can be separated in order to study the fundamental behavior of diffusion flame extinction. With this geometry, reactant is supplied uniformly from the burner into the ambient filled with other reactant. After the ignition,

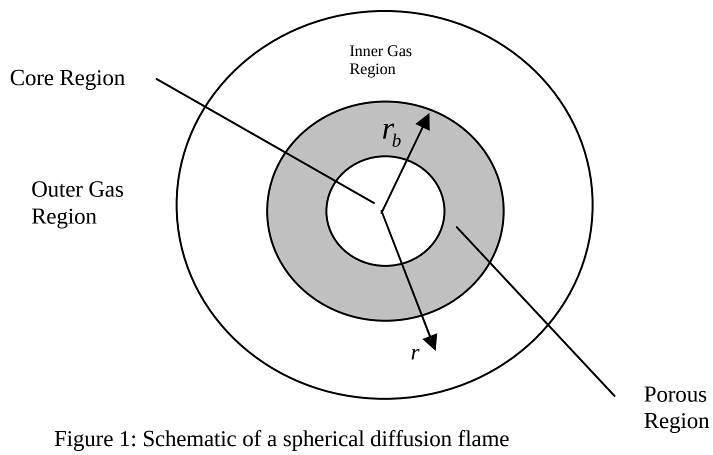

Figure 1: Schematic of a spherical diffusion flame

a spherical flame will propagate out until it is extinguished, steady state is reached, or it establishes a position where fuel and oxygen are totally consumed. The flame is spherical due to lack of gravity in space. One of the advantages of this geometry is being able to control the convection direction from fuel to oxidizer (if fuel in supplied from the burner) or from oxidizer to fuel (if oxygen is supplied from burner). Also, this geometry allows for the control how much the inert gas (primarily nitrogen) will be supplied in the fuel side and how much in the oxygen side.

Due to this geometry, four limiting cases arise: 1. fuel supplied from the burner into an ambient with air; 2. diluted fuel supplied into oxygen; 3. air supplied into fuel; and 4. oxygen supplied into diluted fuel. Existing studies show that Lewis number of the ambient reactant have a strong effect on the flame properties or flame characteristics. Lewis number is the ratio of characteristic mass diffusion and characteristic thermal diffusion. For the first two cases, where oxygen is in the ambient, studies show that Lewis number is close to unity, not giving much insight on how it affects flame properties. When fuel is in ambient, however, Lewis number can be away from one. Therefore, in order to better understand the effect of Lewis number on flame properties, problem where the ambient is filled with fuel, namely ethylene, was studied for the analytical research.

The research studied the above cases with two approaches. The first approach was an analytical investigation which consisted of formulating a set of equations based on the natural laws of mass, species and energy conservations, and then solving the resulting equations by activation energy asymptotics to identify the flame location, flame temperature, and extinction condition. The second approach was a computational study, using a flame code already developed to study the transient behavior of $C_2H_4/O_2/N_2$ flames under various given conditions.

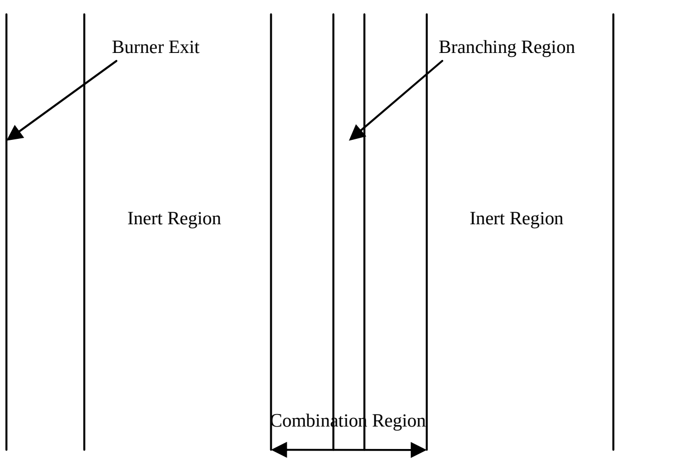

Figure 2: Flow domain split into five regions

Analytical Method

In the analytical investigation, a mathematical formulation that includes the conservation of mass, species concentration, and energy was formulated to identify the flame location, flame temperature, and extinction condition. In the study, the flow domain was split to five subdomains; a very thin branching region in which the branching reaction occurs, two broader but still thin oxidation regions that

sandwich the branching region, and two broad chemically inert transport regions out of the termination regions. Each of these three groups of regions was governed by different transport processes. Equations in each of these regions were solved individually and unified through the matching between two neighboring regions. Radiation was not included so only the kinetic extinction, meaning the limit that reaction rates becoming too slow to support
steady burning, was studied.

In the limit of infinity fast reaction or called reaction-sheet limit, all of the reactants are completely consumed, such that the adiabatic flame temperature given by

$$\tilde{T}_{f,0} = (\tilde{T}_s + \tilde{Y}_{O,s}) - (\tilde{T}_s + \tilde{Y}_{O,s} - \tilde{T}_\infty)[\tilde{Y}_{O,s} / (1 + \tilde{Y}_{O,s})]^{1/Le_F} \qquad (1)$$

is obtained, and the location of the flame sheet is

$$\tilde{r}_f = Le_F \tilde{m} / \ell n (1 + \tilde{Y}_{O,s}{}^{-1}) \qquad (2)$$

In the above, $\tilde{T}_s$ the supplied temperature of the gas at the center of the burner, $\tilde{T}_\infty$ the ambient temperature, $\tilde{Y}_{O,s}$ mass fraction of the oxidizer supplied from the burner, Le_F is the Lewis number of fuel, and $\tilde{m}$ is the mass flow rate. The ~ represent nondimensional quantities defined as such

$$\tilde{T}_r = \frac{c_{p,g} T_r}{q_F Y_{F,\infty}}, \quad \tilde{Y}_O = \frac{\nu_F W_F}{\nu_O W_O} \frac{Y_O}{Y_{F,\infty}}, \quad \tilde{r} = \frac{r}{r_b}, \quad \tilde{m} = \frac{c_{p,g} m}{4\pi r_b \lambda_g} = \frac{4\pi r^2 c_{p,g} \rho_g u}{4\pi r_b \lambda_g} = \frac{r_b^2 \tilde{r}^2 c_{p,g} \rho_g u}{r_b \lambda_g} = (\rho_g u) \tilde{r}^2 \frac{r_b c_{p,g}}{\lambda_g}$$

$$Le_i = \frac{\lambda_g / c_{p,g}}{\rho_g D_i}, \quad \tilde{\rho}_g = \rho_g / \rho_{g,f}$$

where *r* the spatial coordinate along the radial direction (See Figure 1), r_b the outer radius of the porous burner (See Figure 1), T_r the temperature at location *r*, $c_{p,g}$ the specific heat of the gas at constant pressure, $Y_{F,\infty}$ the mass fraction of the fuel at the ambient, Y_O the mass fraction of the oxidizer, q_F heat of combustion per unit mass of the fuel, ν_F the stoichiometric coefficient of the fuel, ν_O stoichiometric coefficient of the oxidizer, W_F the molecular weight of the fuel, W_O the molecular weight of the oxidizer, *m* mass flow rate, *u* radial flow velocity along the radial direction, ρ_g the gas density, $\rho_{g,f}$ gas density at the flame sheet, λ_g the thermal conductivity of the gas, Le_i the Lewis number of species *i* , D_i mass diffusion coefficient of species *i*

To account for finite rate reactions with high activation energies, a simplified two-step reaction mechanism given by

$$\nu_F \, F + R \rightarrow 2\,\mathrm{R} \qquad (3)$$

$$R + \nu_O \, O \rightarrow P \qquad (4)$$

was adopted, where *F* is the fuel, *R* the radical, and *P* the products. Both reactions are of the high activation energy kind. The branching reaction, (3), represents the pyrolysis of fuel molecules for the production of radicals, is a very high activation energy and slightly endothermic reaction. The termination reaction, (4), symbolizing the combination of radicals to produce final combustion products, has relatively lower activation energy but is highly exothermic. Only the chain branching and termination reactions were considered since these two types of reactions will lead to extinction.

Since reaction rates are not infinity fast, a small amount of reactant leakage across the flame and a small flame temperature reduction occur:

The analysis yielded a structure equation

$$d^2\, \Theta_1^{\pm} / d\,\zeta^2 = \Lambda_2\, \Phi_{R,1}^{\pm}\, \Phi_{O,1}^{\pm} \exp(-\Theta_1^{\pm}) \qquad (5)$$

with boundary conditions

$$\Theta_1^{-}(\zeta \rightarrow -\infty) = -\tilde{T}_{b,1} \exp[\tilde{m}(1-\tilde{r}_f^{-1})] - (\tilde{T}_{f,0}-\tilde{T}_s)(\tilde{m}/\tilde{r}_f^{2})\zeta \qquad (6)$$

$$(d\,\Theta_1^{-}/d\zeta)_{\zeta\rightarrow -\infty} = -(\tilde{T}_{f,0}-\tilde{T}_s)(\tilde{m}/\tilde{r}_f^{2}) \qquad (7)$$

$$\Theta_1^{+}(\zeta \rightarrow \infty) = -a_{T,1}^{+}[1-\exp(-\tilde{m}/\tilde{r}_f)] + [\tilde{Y}_{O,s} - (\tilde{T}_{f,0}-\tilde{T}_s)](\tilde{m}/\tilde{r}_f^{2})\zeta \qquad (8)$$

$$(d\,\Theta_1^{+}/d\zeta)_{\zeta\rightarrow \infty} = [\tilde{Y}_{O,s} - (\tilde{T}_{f,0}-\tilde{T}_s)](\tilde{m}/\tilde{r}_f^{2}) \qquad (9)$$

$$\Theta_1^{-}(\zeta = 0) = \Theta_1^{+}(\zeta = 0) = \tilde{T}_{f,1} \qquad (10)$$

$$(d\,\Theta_1^{-}/d\,\zeta)_{\zeta=0} = (d\,\Theta_1^{+}/d\,\zeta)_{\zeta=0} \qquad (11)$$

where Θ_1 the temperature reduction from the adiabatic flame temperature in the reaction region, $\Phi_{R,1}$ is the radical concentration in reaction region, $\Phi_{O,1}$ the oxidizer concentration in reaction region, ζ the stretched coordinate in the reaction region, Λ_2 the reduced *Damköhler* number representing the ratio of the characteristic flow time and the characteristic reaction time, $T_{b,1}$ the deviation of burner exit temperature from the reaction-sheet limit, and $a_{T,1}$ an integration constant representing the temperature decrease from the reaction-sheet limit in the chemically inert region. The expressions of $\Phi^{\pm}_{R,1}$ and $\Phi^{\pm}_{O,1}$ were solved from the analysis as

$$\Phi_{O,1}^{\pm} = Le_O\{\Theta_1^{\pm} + a_{T,1}^{\pm}[1-\exp(-\tilde{m}/\tilde{r}_f)] - (\tilde{T}_s + \tilde{Y}_{O,s} - \tilde{T}_{f,0})(\tilde{m}/\tilde{r}_f^{2})\zeta\} - a_{T,1}^{\pm}[1-\exp(-Le_O\,\tilde{m}/\tilde{r}_f)] \qquad (12)$$

$$\Phi^-_{R,1} = Le_R\{\Theta^-_1 + a^+_{T,1}[1-\exp(-\tilde{m}/\tilde{r}_f)] + (\tilde{T}_{f,0} - \tilde{T}_s)(\tilde{m}/\tilde{r}_f^2)\zeta\} - a^+_{T,1}[1-\exp(-Le_R\,\tilde{m}/\tilde{r}_f)] \quad (13)$$

$$\Phi^+_{R,1} = Le_R\{\Theta^+_1 + a^+_{T,1}[1-\exp(-\tilde{m}/\tilde{r}_f)] - (\tilde{T}_s + \tilde{Y}_{O,s} - \tilde{T}_{f,0})(\tilde{m}/\tilde{r}_f^2)\zeta\} - a^+_{T,1}[1-\exp(-Le_R\tilde{m}/\tilde{r}_f)] \quad (14)$$

where Le_O and Le_R is the Lewis numbers of the oxidizer and reactant, respectively.
Equation (5) subjected to the boundary conditions (6)-(11) needs to be integrated numerically. A code using a fourth order Runge-Kutta Method was developed and the solutions of the T1 (0), representing reduction of the flame temperature from the adiabatic limit, versus the Lamba2Bar ($\bar{\lambda}_2$, rescaled reduced *Damköhler* number) for selected Lewis numbers were obtained. Varying the Lewis number of a reactant while fixing the other's, the reactant's effects on the flame properties were studied. For example, varying fuel's Lewis number while fixing the Lewis numbers of radical and oxidizer, fuel's effects on flame properties were only observed.

Whereas, the analytical analysis examined the steady burning of diffusion flame in microgravity, the numerical method will study the transient behavior.

NUMERICAL METHOD

The computational study was performed using a flame code already developed to study the transient behavior of $C_2H_4/O_2/N_2$. The transient flame responses from the ignition to extinction or steady burning were recorded. The flame code incorporated the description of detailed transport and reaction kinetics to accurately predict the burning characteristics. Because microgravity flames were strongly affected by radiation, a realistic optically thick radiation model was included to study both the kinetic and radiative extinction limits. The radiative extinction limit was a flame extinction state that does not exist without radiation. This limit was first reported by Chao et al. (1991). The flame temperature (maximum temperature within the flow) and flame location (where the maximum temperature is located) were studied versus time and the effects of given conditions including the flow conditions and radiative heat loss were analyzed. Cases with $C_2H_4 \rightarrow$17% O_2 + 83% N_2 with a mass flow rate of 1.51mg/s and 2 mg/s were ran.

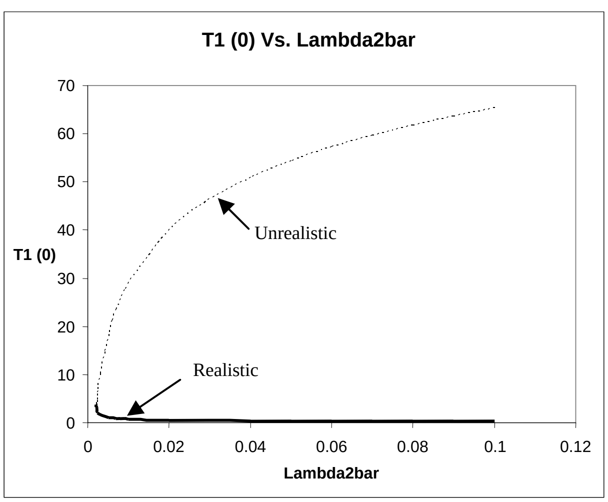

Figure 3: $Le_F = Le_O = Le_R$ =1. The dotted curve is not an unrealistic solution and the solid curve is the true solution.

ANALYTICAL RESULTS

As mention above, the analytical analysis had to be solved numerically and solutions of the T1(0) versus the Lamba2Bar ($\bar{\lambda}_2$) for selected Lewis numbers were obtained. Figure 3 shows a baseline plot where the Lewis numbers of all the reactants are unity ($Le_F = Le_O = Le_R$ =1). It is worth noting that the dotted curve is an unrealistic solution and the solid curve is the true solution. The reason for this is that as Lamda2Bar increases, the reaction rate increases, making reaction more complete. This causes the flame temperature to approach the adiabatic flame temperature,

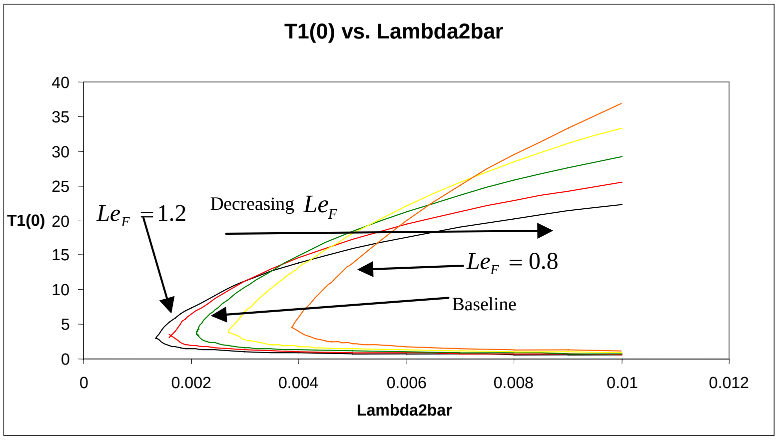

Figure 4: Plots with varying Le_F but fixed Le_R and Le_O

meaning the change in temperature T1(0) approaches zero, in accordance to the solid curve and not the dotted curve. The point where the solid and dotted curves intersect is the smallest possible Lamba2Bar ($\bar{\lambda}_2$) where the flame can still exist and not extinguish, reaching its kinetic extinction state. Beyond this point, there is no solution.

Figure 4 shows curves with different Lewis numbers of fuel but all with Lewis numbers of radical and oxidizer of unity. As shown, it can be seen that the Lewis number has a profound impact on the flame characteristics, especially the flame's kinetic extinction point. The smaller the Lewis number, the smaller the reaction rate it can sustain. This is because as the Lewis number of fuel decreases, mass diffusion increases, increasing the reactant leakage that causes incomplete reaction. This leads the flame to extinguish at a much lower reaction rate. Although the spread from the baseline curve is not as severe as fuel's, by varying the Lewis number of the radical while fixing the Lewis numbers of fuel and oxidizer to unity, again, as Lewis number decreases, the flame goes extinct at a much lower reaction rate (see Figure 5). Finally, by varying the Lewis number of oxidizer while fixing the Lewis numbers of fuel and radical to unity, it is observed in Figure 6 that the kinetic extinction limit does not differ from the baseline, as seen from the previous two cases. The reason for this is because oxidizer is supplied from

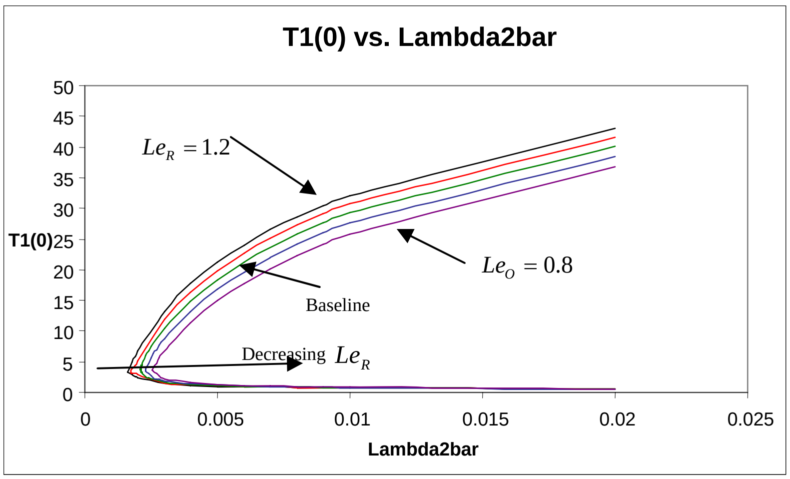

Figure 5: Plots with varying Le_R but fixed Le_F and Le_O

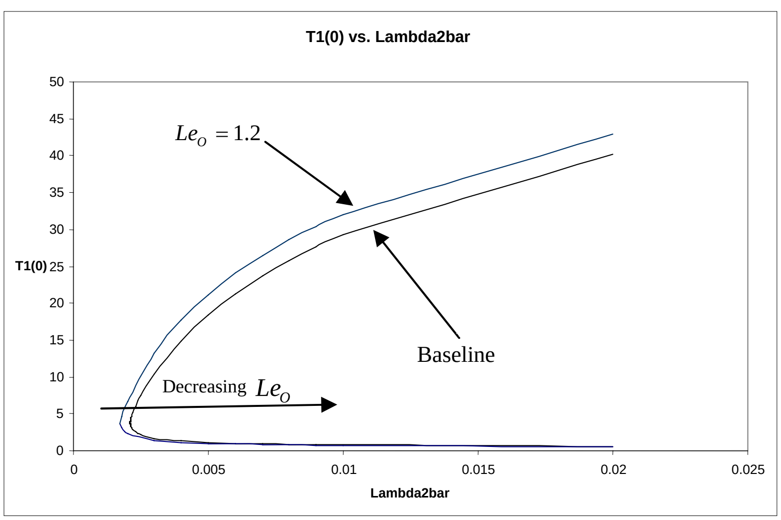

Figure 6: Plot with varying Le_O but fixed Le_R and Le_F

the burner, which causes convection to dominate over mass diffusion.

NUMERICAL RESULTS

Cases with $C_2H_4 \rightarrow$17% O_2 + 83% N_2 with a mass flow rate of 1.51mg/s and 2 mg/s were ran and the transient flame responses from the ignition to extinction or steady burning were recorded. From Figures 7 and 8, it can be seen that extinction of the flame with flow rate of 1.51 and 2.11 mg/s occurs at 3.3 and 1.3 seconds, respectively. The extinction occurs when the radius of the flame and temperature decreases abruptly. The difference in extinction time between the two flow rates is due to radiative heat loss. As flow rate increases, the radius of the flame also increases. After ignition, a spherical flame propagates out, due to the consumption of fuel and oxygen. As this is happening, the temperature of the flame decreases with time, due to the radiative heat loss (see Figure 8). It is known that radiation is a volumetric effect, that is, as the flame gets larger, the greater the heat loss due to radiation, and, therefore, the lower the flame temperature. The temperature will drop to a point where the reaction can no longer be sustained, such that the flame will be extinguished.

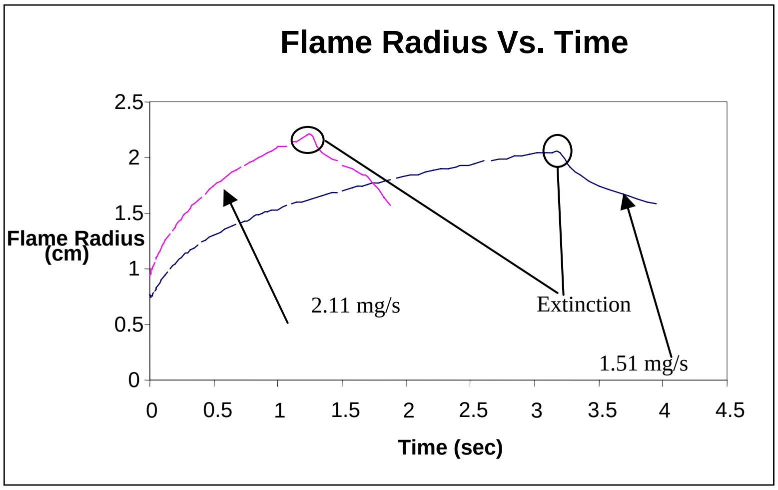

Figure 7: Plots of transient response of flame radius. Plots with flow rates of 1.51 and 2.11 mg/s

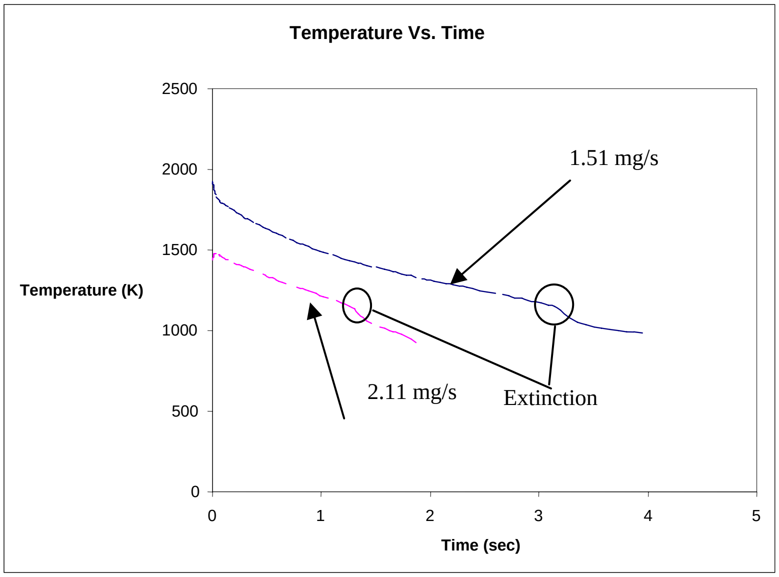

Figure 8: Plots of transient response of flame temperature. Plots with flow rates of 1.51 and 2.11 mg/s

CONCLUSION

From the analytical analysis, it was observed that Lewis number of fuel in the ambient has a profound impact on the kinetic extinction state. By decreasing the Lewis number of fuel, the flame extinguished at a lower reaction rate. From the numerical analysis, it was observed that flames with a higher flow rate extinguish quicker, due to the radiative heat loss experienced as the flame propagated out after ignition.

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REFERENCES

Chao, B. H., Law, C. K. and T'ien, J. S. (1991). Structure and Extinction of Diffusion Flames with Flame Radiation. Twenty-Third Symposium (International) on Combustion, 523-531.

Liu, S., Chao, B. H. and Axelbaum, R. L., (2005). *A Theoretical Study on Soot Inception in Spherical Burner-Stabilized Diffusion Flames,* Combustion and Flame 140, 1-23.