

## Research Article

# Modified Quasi-Steady Fuel Droplet Combustion Model

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The quasi-steady model of the combustion of a fuel droplet has been modified. The approach involved the modification of the quasi-steady model to reflect the difference in constant properties across the flame front. New methods for accurately estimating gas constants and for estimating Lewis number are presented. The proposed theoretical model provides results that correlate favorably with published experimental results. The proposed theoretical model also eliminates the need for unguided adjustment of thermal constants or the complex analysis of the variation of thermal properties with temperature and can serve as a basis for analysis of other combustion conditions like droplets cloud and convective and high-pressure conditions.

## 1. Introduction

Fuel droplet models are used to describe the influence of droplet size and ambient conditions on fuel combustion in devices such as diesel engines, rocket engines, gas turbines, oil fired boilers, and furnaces [1, 2]. The simple quasi-steady model, which is the focus of this paper, has its origin in the 1950s [3, 4] and is widely accepted as the theoretical model of fuel droplet combustion [5]. The important results of this theory are as follows [1, 4–7]:

$$\dot{m} = \frac{4\pi k_g r_s}{c_{pg}} \ln(1 + B), \quad (1)$$

where

$$B = \frac{\Delta h_c / \nu + c_{pg}(T_\infty - T_s)}{q_{i-1} + h_{fg}},$$

$$T_f = \frac{(q_{i-1} + h_{fg})}{c_{pg}(1 + \nu)} [\nu B - 1] + T_s,$$

$$\frac{r_f}{r_s} = \frac{\ln(1 + B)}{\ln(1 + 1/\nu)}, \quad (2)$$

$$D^2 = D_0^2 - Kt,$$

$$t_d = \frac{D_0^2}{K},$$

where

$$K = \frac{8k_g}{\rho_l c_{pg}} \ln(1 + B) = \frac{2\dot{m}}{\pi \rho_l r_s}. \quad (3)$$

Note that though the simple quasi-steady model theory has its roots in the 1950s, it has been developed upon through the 1950s to the 1970s in order to arrive at the results presented above [1–7]. However, simple quasi-steady model provides unsatisfactory results in comparison with several experimental observations [1, 5, 8–12]. The simple quasi-steady model is best at predicting fuel mass flow rate  $\dot{m}$  and the  $d^2$  law but does not accurately predict the flame to droplet radius ratio  $r_f/r_s$  and flame temperature  $T_f$  [5]. The simple quasi-steady model typically predicts  $r_f/r_s$  higher than observed values, and  $T_f$  is usually lower than that experimentally observed. Experiments have also shown that the values of  $r_f/r_s$  and  $T_f$  may not be constant. Law et al. [10] showed that fuel vapor accumulation causes transient effects in the values of  $r_f/r_s$  and  $T_f$ , but Raghunandan and Mukunda [5] later showed that the condensed-phase unsteadiness lasts for 20–25% of burning time and concluded that the discrepancies between experiments and simple quasi-steady model cannot be attributed to condensed-phase unsteadiness. A study by He et al. [8] revealed that the flame front motion has the effect of causing unsteadiness and variation of  $r_f/r_s$  and  $T_f$  during combustion. The analytical model of Raghunandan and Mukunda [5] for quasi-steady droplet combustion

with variable thermodynamic and transport properties, and nonunity Lewis number gave accurate prediction of  $K$  and significant improvement in  $r_f/r_s$  and  $T_f$  compared to the simple quasi-steady model. Puri and Libby [13] used a detailed expression for the heat transfer and transport properties and came up with a complex model of the quasi-steady fuel droplet combustion. Their model is best solved numerically. Filho [14] solved the quasi-steady fuel droplet combustion problem in a way similar to Puri and Libby's solution. Filho's solution was less complicated and involved the removal of nonlinearity in the heat transfer and transport properties coefficients. Imaoka and Sirignano [15–17] solved the fuel droplet combustion problem for the case of a droplet cloud using unity Lewis number assumption. They acknowledged that the use of unity Lewis number significantly overestimates  $r_f/r_s$ . Imaoka and Sirignano [15–17] focused on the variation of constants from one droplet to another in the droplet cloud. The vaporization rate was found for each droplet in the droplet cloud because they assumed that the solutions for each droplet are not equal.

In this paper, the simple quasi-steady fuel droplet combustion model is modified for higher accuracy by assuming discontinuity in the heat transfer and transport coefficients across the flame sheet and nonunity Lewis number for the inner and outer region. A method for estimating property constants for the two regions is recommended. Note that while the discontinuity in Imaoka and Sirignano [15–17] solution is from droplet to droplet, the discontinuity assumed in this paper is from the inner region to the outer region of a burning droplet.

## 2. Method

In the derivation of the classical droplet combustion model, the following assumptions are made [1, 4–7].

- (i) Burning droplet is spherical and surrounded by a spherically symmetric flame in a quiescent infinite medium.
- (ii) Burning process is quasi-steady.
- (iii) Fuel is a single component and pressure is uniform and constant.
- (iv) Gaseous species are of 3 types: fuel vapor, oxidizer, and combustion products.
- (v) Stoichiometric proportions of fuel-oxidizer are at flame.
- (vi) Unity Lewis number is assumed.
- (vii) Radiation heat transfer is negligible.
- (viii) No soot or liquid water is present.
- (ix) Uniform species thermal constants:  $c_p$  and  $k$ .

These assumptions are good, but the following assumptions changes will be made in order to improve the accuracy of the model.

- (i) Unity Lewis is assumed only at the source of diffusing species, and nonunity Lewis number is assumed in

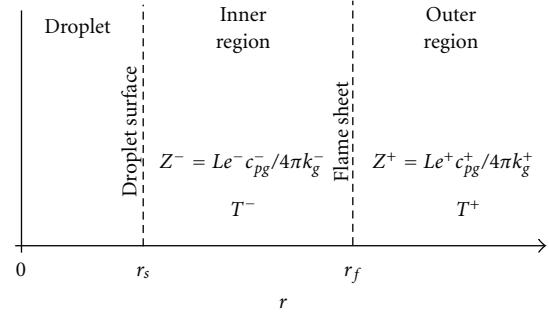


FIGURE 1: Separation of inner region and outer region species properties.

the outer and inner regions. This assumption is made because, at the sources of diffusing specie, the generation of the diffusing specie causes the thermal diffusivity to balance the mass diffusivity, while, away from the source of diffusing species, the thermal diffusivity and mass diffusivity have different values depending on the species concentration, species properties, and temperature profile.

- (ii) The property of the inner region is different from the property of the outer region. This assumption is made because the average temperature in the outer region is different from the average temperature in the inner region and the species composition in the outer region is different from the species composition in the inner region.

The new assumption that the property of the inner region is different from the property of the outer region is shown in Figure 1. This new assumption makes it necessary to have two average temperatures since there are two different sets of temperature extremes in the two regions.

In order to relate the outer constants to the inner constants, let

$$Z^+ = nZ^-, \quad (4)$$

where  $n$  is a constant and (4) implies that

$$n = \frac{Le^+ c_{pg}^+ k_g^-}{Le^- c_{pg}^- k_g^+}. \quad (5)$$

The mass flow rate,  $\dot{m}$ , is treated as a constant and independent of radius,  $r$ , since quasi-steady burning is assumed. In the inner region, Fick's law can be presented in the form [1]

$$\dot{m}|_{\text{fuel}} = -4\pi r^2 \frac{\rho \mathcal{D}}{1 - Y_F} \frac{dY_F}{dr} \quad (6)$$

with boundary conditions (BCs)

$$\begin{aligned} Y_F(r_s) &= Y_{F,s}(T_s), \\ Y_F(r_f) &= 0. \end{aligned} \quad (7)$$

Integration of (6) and application of BCs (7) gives

$$Y_{F,s} = 1 - \frac{\exp(-Z^- \dot{m}/r_s)}{\exp(-Z^- \dot{m}/r_f)}, \quad (8)$$

where  $Z = 1/4\pi\rho\dot{D} = Le \cdot c_{pg}/4\pi k_g$ .

In the outer region, Fick's law in terms of the constant fuel mass flow rate can be presented in the form [1]

$$\dot{m}|_{\text{fuel}} = -4\pi r^2 \frac{\rho\dot{D}}{v - Y_{Ox}} \frac{dY_{Ox}}{dr} \quad (9)$$

with BCs

$$\begin{aligned} Y_{Ox}(r_f) &= 0, \\ Y_{Ox}(r \rightarrow \infty) &= 1. \end{aligned} \quad (10)$$

Integration of (9) and application of BCs (10) gives the relation between  $\dot{m}$  and  $r_f$  as

$$\exp\left(\frac{Z^+ \dot{m}}{r_f}\right) = \frac{v+1}{v}. \quad (11)$$

Equation (4) in (11) gives

$$\exp\left(\frac{nZ^- \dot{m}}{r_f}\right) = \frac{v+1}{v}. \quad (12)$$

In order to find the temperature profiles in the inner and outer region, the Shvab-Zeldovich form of the energy equation [1] is used, that is,

$$\frac{d(r^2(dT/dr))}{dr} = Z\dot{m} \frac{dT}{dr} \quad (13)$$

with two sets of BCs for the inner and outer regions

$$\begin{aligned} \text{BC}^- &\begin{cases} T(r_s) = T_s \\ T(r_f) = T_f, \end{cases} \\ \text{BC}^+ &\begin{cases} T(r_f) = T_f, \\ T(r \rightarrow \infty) = T_\infty. \end{cases} \end{aligned} \quad (14)$$

Integration of (13) and application of inner region BCs (14) gives

$$\begin{aligned} T^-(r) &= \frac{(T_s - T_f) \exp(-Z^- \dot{m}/r) + T_f \exp(-Z^- \dot{m}/r_s) - T_s \exp(-Z^- \dot{m}/r_f)}{\exp(-Z^- \dot{m}/r_s) - \exp(-Z^- \dot{m}/r_f)} \end{aligned} \quad (15)$$

for the inner region and

$$T^+(r) = \frac{(T_f - T_\infty) \exp(-Z^+ \dot{m}/r) + T_\infty \exp(-Z^+ \dot{m}/r_f) - T_f}{\exp(-Z^+ \dot{m}/r_f) - 1} \quad (16)$$

for the outer region, and (4) into (16) gives

$$\begin{aligned} T^+(r) &= \frac{(T_f - T_\infty) \exp(-nZ^- \dot{m}/r) + T_\infty \exp(-nZ^- \dot{m}/r_f) - T_f}{\exp(-nZ^- \dot{m}/r_f) - 1}. \end{aligned} \quad (17)$$

At the surface of the droplet, the heat conducted to it balances the heat used to vaporize and heat up the droplet. Hence, the energy balance at the droplet surface [1] can be written in the form

$$k_g^- 4\pi r_s^2 \frac{dT^-}{dr} \Big|_{r_s} = \dot{m} (h_{fg} + q_{i-1}). \quad (18)$$

Differentiating (15) and substituting into (18) give the energy balance at the droplet as

$$\frac{4\pi k_g^- Z^- (T_f - T_s)}{(q_{i-1} + h_{fg})} \cdot \frac{\exp(-Z^- \dot{m}/r_s)}{[\exp(-Z^- \dot{m}/r_s) - \exp(-Z^- \dot{m}/r_f)]} + 1 = 0. \quad (19)$$

At the flame sheet, the heat of combustion is conducted away by both the inner region and outer region gases. Therefore, the energy balance at the flame sheet can be written in the form [1]

$$\dot{m} \Delta h_c = k_g^- 4\pi r_f^2 \frac{dT^-}{dr} \Big|_{r_f} - k_g^+ 4\pi r_f^2 \frac{dT^+}{dr} \Big|_{r_f}. \quad (20)$$

Differentiating (15) and (17) and substituting into (20) give the simplified energy balance at the flame sheet as

$$\begin{aligned} 1 &= \frac{4\pi}{\Delta h_c} \cdot \frac{k_g^- Z^- (T_f - T_s) \exp(-Z^- \dot{m}/r_f)}{[\exp(-Z^- \dot{m}/r_s) - \exp(-Z^- \dot{m}/r_f)]} \\ &\quad - \frac{4\pi}{\Delta h_c} \cdot \frac{k_g^+ nZ^- (T_\infty - T_f) \exp(-nZ^- \dot{m}/r_f)}{[1 - \exp(-nZ^- \dot{m}/r_f)]}. \end{aligned} \quad (21)$$

Solving (12), (19), and (21) for  $\dot{m}$ ,  $r_f$ , and  $T_f$  gives

$$\begin{aligned} \dot{m} &= \frac{4\pi k_g^- r_s}{Le^- c_{pg}} \\ &\quad \times \left\{ \ln \left[ \frac{1}{1 + (k_g^- / n\nu k_g^+)} \right] \right. \\ &\quad \left. + \frac{(T_\infty - T_s) Le^- c_{pg} / (1 + (k_g^- / n\nu k_g^+)) + \Delta h_c / ((n\nu k_g^+ / k_g^-) + 1)}{(q_{i-1} + h_{fg})} \right\} \\ &\quad + \frac{1}{n} \ln \left[ \frac{v+1}{v} \right] \Bigg\}. \end{aligned} \quad (22)$$

Let

$$A = \frac{1}{1 + (k_g^-/nvk_g^+)} \cdot \left(\frac{v+1}{v}\right)^{1/n},$$

$$B = \frac{(T_\infty - T_s)Le^-c_{pg}^- / (1 + (k_g^-/nvk_g^+)) + \Delta h_c / ((nvk_g^+/k_g^-) + 1)}{(q_{i-1} + h_{fg})} \cdot \left(\frac{v+1}{v}\right)^{1/n},$$
(23)

then

$$\dot{m} = \frac{4\pi k_g^- r_s}{Le^-c_{pg}^-} \ln(A+B),$$

$$T_f = \frac{(q_{i-1} + h_{fg})}{Le^-c_{pg}^-} \left[ (A+B) \cdot \left(\frac{v}{v+1}\right)^{1/n} - 1 \right] + T_s,$$

$$\frac{r_f}{r_s} = \frac{n \ln(A+B)}{\ln[(v+1)/v]}.$$
(25)

The new mass flow rate from (24) was used to obtain burning constant and droplet life time as

$$K = \frac{8k_g^-}{\rho l c_{pg}^- Le^-} \ln(A+B),$$

$$t_d = \frac{D_0^2}{K}.$$
(26)

### 3. Estimation of Thermal Property Constants

The species properties for the inner region are estimated as follows:

$$\bar{T}^- = 0.5(T_s + T_f),$$
(27)

$$k_g^- = 0.4k_F(\bar{T}^-) + 0.6k_{Ox}(\bar{T}^-),$$
(28)

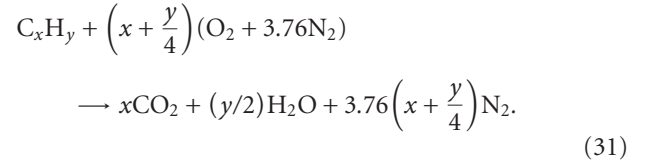
$$c_{pg}^- = Y_F^- c_{pF}(\bar{T}^-) + Y_{Ox}^- c_{pOx}(\bar{T}^-).$$
(29)

Equation (27) is average temperature in the inner region. Equation (28) has been directly adapted from law and William's suggestion [9, 18] since it was experimentally derived, and it replaces the complex estimation of thermal conductivity for a mixture of gas. Equation (29) is the specific heat constant of the gaseous mixture in the inner region. The mass fractions in (29) are estimated by assuming a linear fuel mole fraction from the fuel surface to the region close to the flame where there is a stoichiometric mixture of fuel and oxidizer. Therefore, at the fuel droplet surface,

$$\chi_{F,s} \approx 1,$$

$$\chi_{Ox,s} \approx 0.$$
(30)

At the region close to the flame and for the case of hydrocarbon fuel droplet combustion in air, the reaction equation is typically



The mole fractions can be estimated from the reactants as

$$\chi_{F,r_f^-} = \frac{1}{1+x+y/4},$$

$$\chi_{Ox,r_f^-} = \frac{x+y/4}{1+x+y/4}.$$
(32)

Therefore, the average mole fractions for the inner region are

$$\chi_F^- = 0.5(\chi_{F,s} + \chi_{F,r_f^-}) = 0.5 + \frac{0.5}{1+x+y/4},$$

$$\chi_{Ox}^- = 0.5(\chi_{Ox,s} + \chi_{Ox,r_f^-}) = \frac{0.5x+y/8}{1+x+y/4}.$$
(33)

The mole fractions can then be used to estimate the mass fractions

$$Y_F^- = \frac{\chi_F^- M_F}{\chi_F^- M_F + \chi_{Ox}^- M_{Ox}},$$

$$Y_{Ox}^- = \frac{\chi_{Ox}^- M_{Ox}}{\chi_F^- M_F + \chi_{Ox}^- M_{Ox}}.$$
(34)

And the specie constants for the outer region are estimated as follows:

$$\bar{T}^+ = 0.5(T_\infty + T_f),$$

$$c_{pg}^+ = c_{pOx}(\bar{T}^+),$$

$$k_g^+ = k_{Ox}(\bar{T}^+).$$
(35)

The oxidizer (which is usually air) mainly dominates the outer region, so the outer region constants are evaluated directly from the oxidizer properties. Additionally, it is reasonable to assume that  $q_{i-1} = 0$  and  $T_s = T_{boil}$ , since the droplet is burning vigorously after an initial transient heat up.

### 4. Estimation of Lewis Number

For the estimation of Lewis number in the two regions, unity Lewis number is assumed at the source of diffusing specie. Therefore, in the inner region where fuel diffuses from the droplet surface, unity Lewis number is assumed at the droplet surface

$$Le^-(T_s) = 1.$$
(36)

By definition,

$$Le^- = \frac{\alpha^-}{\mathcal{D}^-}. \quad (37)$$

Assuming ideal-gas behavior, the pressure and temperature dependence of diffusion coefficient [19] is given as

$$\mathcal{D} \propto \frac{T^{3/2}}{P} \quad (38)$$

which implies that

$$\mathcal{D} = C \frac{T^{3/2}}{P} = CT^{3/2}, \quad (39)$$

where  $C$  is a constant to be found and  $P$  has been absorbed into the constant because the combustion takes place at constant pressure. By applying the boundary condition  $Le^-(T_s) = 1$ ,  $C$  is found as

$$C = \frac{\alpha^-(T_s)}{T_s^{3/2}}. \quad (40)$$

Combining (40), (39), and (37) gives

$$Le^- = \frac{\alpha^-(\bar{T}^-)}{\alpha^-(T_s)} \cdot \left( \frac{T_s}{\bar{T}^-} \right)^{3/2}, \quad (41)$$

where

$$\alpha^-(T_s) = \frac{k_F(T_s)}{\rho_{F\text{-vapor}}(T_s) \cdot c_{pF}(T_s)}. \quad (42)$$

Fuel dominates at the vapor-surface interface, so density is estimated as

$$\rho_{F\text{-vapor}}(T_s) = \frac{P}{T_s R_F} = \frac{P}{T_s \cdot (R_u/M_F)}, \quad (43)$$

$$\alpha^-(\bar{T}^-) = \frac{k_g^-}{\rho^- \cdot c_{pg}^-},$$

where  $k_g^-$  and  $c_{pg}^-$  are given by (28) and (29), and  $\rho^-$  is estimated as

$$\rho^- = \frac{P}{\bar{T}^- R^-} = \frac{P}{\bar{T}^- \cdot (R_u/M^-)}, \quad (44)$$

with

$$M^- = Y_F^- M_F + Y_{Ox}^- M_{Ox}. \quad (45)$$

Secondly, in the outer region where the combustion products diffuse from the flame sheet, so unity Lewis number is assumed at the flame sheet

$$Le^+(T_f) = 1. \quad (46)$$

Using estimation method similar to that done for the inner region gives

$$Le^+ = \frac{\alpha^+(\bar{T}^+)}{\alpha^+(T_f)} \cdot \left( \frac{T_f}{\bar{T}^+} \right)^{3/2}. \quad (47)$$

At the flame sheet, the mixture fractions can be estimated from the reaction equation ((31) for the combustion of  $C_xH_y$  droplet in air).  $\alpha$ s in (47) are estimated as

$$\alpha^+(T_f) = \frac{k_{\text{Product}}(T_f)}{\rho_{\text{Product}}(T_f) \cdot c_{p\text{Product}}(T_f)}, \quad (48)$$

$$\alpha^+(\bar{T}^+) = \frac{k_g^+}{\rho^+ \cdot c_{pg}^+}.$$

For the case of combustion in air,  $N_2$  dominates the product and outer region, and the property of air can be used to estimate  $\alpha$ s

$$Le^+ \approx \frac{\alpha_{\text{Air}}(\bar{T}^+)}{\alpha_{\text{Air}}(T_f)} \cdot \left( \frac{T_f}{\bar{T}^+} \right)^{3/2}. \quad (49)$$

Equation (49) provides a valid approximation for Lewis number of the outer region and is recommended, since tabulated values of  $\alpha_{\text{Air}}$  are readily available [1, 20–23].

## 5. Results and Discussions

As an example, calculation of combustion variables for the case of  $n$ -heptane ( $C_7H_{16}$ ) droplet combustion in air was done. Both the simple quasi-steady model and the proposed new model (modified quasi-steady model) were used. Ambient conditions were used, that is,  $P = 1$  atm and  $T_\infty = 298$  K. It was assumed that  $T_s = T_{\text{boil}}$ , and droplet heating is negligible, that is,  $q_{i-1} = 0$ .  $T_s = T_{\text{boil}}$  is assumed because it has been experimentally observed that the droplet boils vigorously during the combustion after an initial and brief heatup, and the heat used to heat the droplet from its initial temperature,  $q_{i-1}$ , is usually negligible and has negligible effect on the model result [1, 2]. Initial guess used for  $T_f$  is 2100 K since tabulated values of adiabatic flame temperature of common hydrocarbon fuels are approximately 2000 K.

The calculation results using the simple quasi-steady model are given in Table 1. Law and Williams's suggestion was used to evaluate species properties for use in the simple quasi-steady model [1, 9, 18], and the results for each iteration step are presented. Iteration was repeated till the solution converged to a difference of 2 K or less between the guess flame temperature and the calculated flame temperature. Similarly, results obtained by using the proposed new model are presented in Table 2. Additionally, calculation results for the case of combustion of hexane droplet in ambient conditions using the proposed new model are shown in Table 3. The sample calculations showed that proposed new model predicts realistic flame temperature, evaporation constant, and flame to droplet radius ratio compared to the simple quasi-steady model. In the next section, the results of the proposed new model will be compared to experimental results published.

TABLE 1: Simple quasi-steady model *n*-heptane results.

Iteration	$T_{fG}$ [K]	$\bar{T}$ [K]	$k_{Ox}$ [W/m $\cdot$ K]	$k_F$ [W/m $\cdot$ K]	$k_g$ [W/m $\cdot$ K]	$c_{pF}$ [kJ/kg $\cdot$ K]	$B$	$T_f$ [K]	$r_f/r_s$	$K$ [10 $^3$ cm $^2$ /s]	$ T_{fg}-T_f $ [K]
1	2100	1235.8	0.079415	0.107941	0.090825	4.1634	8.46	968.9	35.00	5.73	1131.1
2	968.9	670.2	0.053133	0.053444	0.053258	3.0872	8.71	1201.2	35.40	4.59	232.3
3	1201.2	786.4	0.056942	0.068886	0.061720	3.3730	8.64	1125.1	35.30	4.85	76.1
4	1125.1	748.3	0.055603	0.063637	0.058817	3.3013	8.66	1142.9	35.32	4.73	17.8
5	1142.9	757.2	0.055909	0.064849	0.059485	3.3030	8.66	1142.5	35.32	4.78	0.4

Fixed variables:  $T_s = T_{boil} = 371.5$  K,  $T_\infty = 298$  K,  $\rho_l = 684$  kg/m $^3$ ,  $\Delta h_c = 44926$  kJ/kg,  $h_{fg} = 316$  kJ/kg, and  $\nu = 15.08$ .

TABLE 2: Proposed model *n*-heptane results.

Iteration	$T_{fG}$ [K]	$\bar{T}^-$ [K]	$k_g^-$ [W/m $\cdot$ K]	$c_{pg}^-$ [kJ/kg $\cdot$ K]	$\bar{T}^+$ [K]	$k_g^+$ [W/m $\cdot$ K]	$c_{pg}^+$ [kJ/kg $\cdot$ K]	$Le^-$	$Le^+$	$n$	$A$	$B$	$T_f$ [K]	$r_f/r_s$	$K$ [10 $^3$ cm $^2$ /s]	$ T_{fG}-T_f $ [K]
1	2100	1235.7	0.090857	3.5920	1199.0	0.077116	1.1739	1.73	0.82	0.18	0.996	58.9	2474.8	11.62	7.00	374.8
2	2474.8	1423.1	0.101818	3.7666	1386.4	0.089698	1.2083	1.72	0.75	0.16	1.017	67.1	2542.8	10.37	7.75	68
3	2542.8	1457.1	0.103923	3.7945	1420.4	0.092212	1.2145	1.72	0.73	0.15	1.022	68.9	2556.2	10.14	7.89	13.4
4	2556.2	1463.8	0.104341	3.7999	1427.1	0.092714	1.2157	1.73	0.73	0.15	1.023	69.3	2558.7	10.09	7.92	2.5
5	2558.7	1465.1	0.104422	3.8009	1428.4	0.092811	1.2160	1.73	0.73	0.15	1.023	69.3	2559.2	10.09	7.93	0.5

Fixed variables:  $T_s = T_{boil} = 371.4$  K,  $T_\infty = 298$  K,  $\rho_l = 684$  kg/m $^3$ ,  $\Delta h_c = 44907$  kJ/kg,  $h_{fg} = 316$  kJ/kg,  $\nu = 15.08$ ,  $\chi_F^- = 0.54$ ,  $\chi_{Ox}^- = 0.46$ ,  $Y_F^- = 0.81$ ,  $Y_{Ox}^- = 0.19$ .

TABLE 3: Proposed model *n*-hexane results.

Iteration	$T_{fG}$ [K]	$\bar{T}^-$ [K]	$k_g^-$ [W/m $\cdot$ K]	$c_{pg}^-$ [kJ/kg $\cdot$ K]	$\bar{T}^+$ [K]	$k_g^+$ [W/m $\cdot$ K]	$c_{pg}^+$ [kJ/kg $\cdot$ K]	$Le^-$	$Le^+$	$n$	$A$	$B$	$T_f$ [K]	$r_f/r_s$	$K$ [10 $^3$ cm $^2$ /s]	$ T_{fG}-T_f $ [K]
1	2100	1221.0	0.106872	2.6318	1199.0	0.077116	1.1739	2.80	0.82	0.18	0.95	63.43	2349.1	11.79	7.32	249.1
2	2349.1	1345.6	0.114822	3.0807	1323.6	0.085242	1.1968	2.45	0.77	0.17	0.96	68.46	2387.7	10.95	7.83	38.6
3	2387.7	1364.9	0.116093	3.1512	1342.9	0.086586	1.2003	2.41	0.76	0.16	0.96	69.38	2394.6	10.81	7.91	6.9
4	2394.6	1368.3	0.116320	3.1638	1346.3	0.086827	1.2010	2.40	0.76	0.16	0.96	69.54	2395.8	10.79	7.92	1.2

Fixed variables:  $T_s = T_{boil} = 342$  K,  $T_\infty = 298$  K,  $\rho_l = 659$  kg/m $^3$ ,  $\Delta h_c = 45091$  kJ/kg,  $h_{fg} = 355$  kJ/kg,  $\nu = 15.2$ ,  $\chi_F^- = 0.55$ ,  $\chi_{Ox}^- = 0.45$ ,  $Y_F^- = 0.79$ ,  $Y_{Ox}^- = 0.21$ .

TABLE 4: Proposed model *n*-heptane results compared with published experimental observations.

	Experimental results [2, 3, 9, 24–27] $P = 1$ atm and $T_\infty = 293$ –300 K	Proposed model $P = 1$ atm and $T_\infty = 298$ K	1999 model [14] $P = 1$ atm and $T_\infty = 298$ K	1991 model [13] $P = 1$ atm and $T_\infty = 298$ K	1950s–1970s model [1–7] $P = 1$ atm and $T_\infty = 298$ K
$T_f$ (K)	2305	2559.2	2631	2631	1142.5
$K$ (10 $^3$ cm $^2$ /s)	7.2–11.4	7.93	14.4	7.9	4.74
$r_f/r_s$	3–10	10.09	33.2	9	35.2

## 6. Comparison with Published Experimental Results

The proposed new model calculation results are compared favorably with published experimental results on the combustion of *n*-heptane. These experimental results and other models calculation results for the combustion of an *n*-heptane droplet in air are summarized in Table 4.

The proximity between calculated and measured values has been greatly improved by the new model proposed in this paper. The proposed new model accurately predicts  $K$  and  $r_f/r_s$ . It predicts  $T_f$  slightly higher and yet closer to

the experimentally observed range compared to previous models. The proposed new model also predicted flame temperature closer to the values predicted by the 1999 and 1991 models compared to the original simple quasi-steady model of the 1950s. The  $K$  and  $r_f/r_s$  values obtained for the combustion of *n*-hexane and *n*-heptane were approximately equal, while  $T_f$  for *n*-heptane was slightly higher than that for hexane.

The estimated flame temperature seems to have the greatest error, and the most probable source of error is in the estimation of  $k_f$ .  $k_f$  at  $\bar{T}^-$  was estimated by extrapolation, which is not good for estimating thermal conductivity of



vapor, because the available data used ranged up to 1000 K only. However, since the estimation of flame temperatures by the newest models is approximately 2600 K, the error may come from experimental error since it may be more difficult to capture the spiked temperature of the flame sheet.

Most of the available tabulated fuel vapor thermal conductivities ranges up to 500 K, and this points out the need for having thermal conductivities tables or curve fits that ranges up to 1500 K or higher in order to use and achieve results with less error.

## 7. Conclusions

The simple quasi-steady model of a fuel droplet was modified to reflect the difference in constant properties across the flame sheet. Two average temperatures were used: one for the inner region and the other for the outer region. The two average temperatures were used to evaluate the assumed constant specific heat and thermal conductivities for the two regions. Nonunity Lewis number was assumed for the two regions while unity Lewis number was assumed at the source of diffusing species, which implies that unity Lewis number was assumed at the flame sheet for the outer region and at the liquid-vapor interface for the inner region. The Lewis numbers obtain in the sample calculation falls within the range that has been observed experimentally [5]. Sample calculations and comparison with experimental results showed that the new model accurately modeled the droplet combustion than the simple quasi-steady model. The new model performance shows that the quasi-steady model of fuel droplet combustion when appropriately applied is a good approximation of the combustion results. The new model also eliminates the need for unguided adjustment of thermal constants and eliminates the need for complex analysis of specific heat and thermal conductivity variation with temperature. The proposed new model is slightly more complex than the original simple quasi-steady model; however, it does not require complex numerical computation for its solutions. The result of the theoretical models of the droplet combustion is best estimated by iteration as shown in the sample calculations. The new model was derive following the process used to derived the old model; hence, it can be noted that if  $n = 1$ ,  $c_{pg}^+ = c_{pg}^- = c_{pg}$ ,  $k_g^+ = k_g^- = k_g$ , and  $Le^+ = Le^- = 1$  are substituted into the new model equations, the old quasi-steady model will be obtained. The new model can serve as a basis for analysis of other droplet combustion conditions like droplet cloud and convective and high pressure conditions.

## Symbols Used

$A$ : Smaller transfer number ( $\sim 1$ )  
 $B$ : Transfer or Spalding number  
 $c_{pg}$ : Specific heat constant of gas [J/kg·K]  
 $C$ : Constant  
 $D$ : Droplet diameter [m]  
 $\mathcal{D}$ : Mass diffusivity [m<sup>2</sup>/s]  
 $h_{fg}$ : Latent heat of vaporization [J/kg]

$K$ : Evaporation rate constant [m<sup>2</sup>/s]  
 $k_g$ : Thermal conductivity of gas [W/m·K]  
 $M$ : Molecular weight [kg/kmol]  
 $\dot{m}$ : Fuel mass flow rate [kg/s]  
 $Le$ : Lewis number  
 $n$ : Constant: Z ratio  
 $P$ : Pressure [atm]  
 $q_{i-l}$ : Interface to liquid heat transfer per unit mass (droplet heating) [J/kg]  
 $R$ : Gas constant [J/Kg·K]  
 $r$ : Radius [m]  
 $T$ : Temperature [atm]  
 $t$ : Time [s]  
 $t_d$ : Droplet life time [s]  
 $x$ : Number of carbon atoms in fuel molecule  
 $Y$ : Mass fraction [kg/kg]  
 $y$ : Number of hydrogen atoms in fuel molecule  
 $Z$ :  $Le \cdot c_{pg}/4\pi k_g$  [m·s/kg]  
 $\Delta h_c$ : Enthalpy of combustion [J/kg]  
 $\alpha$ : Thermal diffusivity [m<sup>2</sup>/s]  
 $v$ : Oxidizer-to-fuel stoichiometric mass ratio [kg/kg]  
 $\rho$ : Density [kg/m<sup>3</sup>]  
 $\chi$ : Mole fraction [kmol/kmol].

## Superscripts

+: Outer region  
 -: Inner region.

## Subscripts

0: Initial condition  
 $\infty$ : Free stream—far from surface  
 boil: Boiling point  
 $d$ : Droplet  
 $f$ : Flame  
 $F$ : Fuel  
 $g$ : Gas  
 $G$ : Guess  
 $i$ : Interface  
 $l$ : Liquid  
 Ox: Oxidizer  
 $s$ : Droplet surface  
 $u$ : Universal.

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