# Solution of a droplet combustion process using modified thermal resistors model

Yoash Mor\* and Alon Gany\*\* \* Ph.D. Student, Faculty of Aerospace Engineering, Technion - Israel Institute of technology yoashmor@gmail.com \*\* Professor Emeritus, Faculty of Aerospace Engineering, Technion - Israel Institute of technology, gany@tx.technion.ac.il

# Abstract

This paper presents a solution to the problem of droplet combustion, using a novel modified thermal resistors model (MTRM). The MTRM can treat heat transfer situations which involve heat sources from chemical reactions or phase transition, such as combustion problems. Its solution for the droplet combustion process yields results which are similar to those of the classical model, but in a simpler way. The MTRM is a powerful analytical technique allowing consideration of multiple heat transfer mechanisms and avoiding certain simplifying assumptions. Thus, it enables solving problems that could not be solved before analytically, obtaining better results.

# 1. Nomenclature

- A Clausius-Clapeyron constant [Pa]
- *B* Clausius-Clapeyron constant [K]
- $c_p$  Specific heat [J/kg K]
- D Mass diffusivity  $[m^2/s]$
- $h_{f_{g}}$  Latent heat of vaporization [J/kg]
- $\Delta h_c$  Heat of combustion [J/kg]
- *k* Thermal conductivity [W/(m K)]
- $\dot{m}$  Mass flow rate [kg/s]
- MW Molecular weight [kg/kmol]
- P Pressure [Pa]
- $\dot{Q}$  Heat transfer rate [W]
- r Radius [m]
- T Temperature [K]
- $\chi$  Mass fraction
- $Y_{F,l}$  Fuel mass fraction at the droplet surface
- *ε* Emissivity
- *v* Oxidizer to fuel stoichiometric ratio [kg/kg]
- $\rho$  Gas mean density [kg/m<sup>3</sup>]
- $\sigma$  Stefan-Boltzmann constant = 5.67  $\cdot 10^{-8}$  W/m<sup>2</sup> K<sup>4</sup>
- $\kappa$  Absorption coefficient [m<sup>-1</sup>]

### **Subscripts**

- b Boiling
- d Droplet
- F Fuel
- f Flame
- g Gas
- *i* Initial
- l Liquid

- *Ox* Oxidizer
- pr Combustion products
- r Radial direction
- $\infty$  Infinity

#### 2. Introduction

The thermal resistance concept is a powerful tool, allowing a simplified solution of one dimensional, constant property, quasi-steady heat transfer problems with no internal heat sources. Furthermore, it enables solving relatively quickly, complex heat transfer problems, including situations involving a number of simultaneous heat transfer mechanisms (for further explanation see Ref. [1]).

Therefore, the motivation for expanding the classical thermal resistance model (CTRM) to other cases is clear. We introduce a modified thermal resistance model (MTRM) expanding the CTRM to situations involving internal chemical heat generation sources, such as chemical reactions or liquid-vapor phase transition.

Like the CTRM, the MTRM describes each heat transfer mechanisms by an analog thermal resistor. The thermal resistor is defined as the temperature difference divided by heat transfer rate of the specific mechanism, i.e.

$$R_{1\to 2} \equiv \frac{T_1 - T_2}{\vec{Q}_{1\to 2}}$$
(1)

where the numbers 1 and 2 denote the upstream and downstream locations along the heat transfer axis. Four types of thermal resistors are defined: radiation, convection, conduction (in media with no internal mass diffusion), and a new coupled thermal resistor that stands for conduction and enthalpy flow in the gas phase (CEF thermal resistor). Illustrations of the possible heat transfer mechanisms and their respective thermal resistors appear in Figures 1 and 2 (adapted from Mor and Gany [2], who also elaborate on the MTRM concept).

According to the MTRM formulation, the energy balance equation equalizes the overall energy flow rates of both sides of each heat source sheet, but rather than writing their explicit form, it presents each local net heat flow rate as the local temperature difference divided by an effective thermal resistance. The effective thermal resistance in each region stands for all the various heat transfer mechanisms that prevail there (or their representative thermal resistances), and it is calculated according to the same summation rules of the CTRM.



Figure 1: schematic illustration of the various energy flow and heat transfer mechanisms around a phase transition interface and a flame/chemical reaction sheet (after [2]).



Figure 2: schematic illustration of the various possible thermal resistors around a phase transition interface and a flame/chemical reaction sheet (after [2]).

In the following sections we will briefly introduce the development of the new CEF thermal resistor in spherical coordinates, and then apply it to a burning n-heptane droplet.

## 3. A development of the CEF thermal resistor in spherical coordinates

The heat transfer rate of the coupled heat transfer mechanism of conduction and enthalpy flow rate is:

$$\vec{\dot{Q}}_{CEF} = \vec{\dot{Q}}_{Cond} + \vec{\dot{Q}}_{EF} = -4\pi k r^2 \frac{dT}{dr} + \sum_j \vec{m}_j h_{f,j}$$
(2)

Where *j* denotes all the species in the represented region. Assuming a simple temperature dependence of the enthalpy:  $h_j = h_j^o + c_p \left(T - T_{ref}\right)$ , equation (2) becomes:

$$\vec{\dot{Q}}_{CEF} = -4\pi kr^2 \frac{dT}{dr} + \sum_j \vec{m}_j \left[ h_{f,j}^o + c_{p,j} \left( T - T_{ref} \right) \right]$$
(3)

 $\dot{Q}_{CEF}$  is constant because it prevails in region with no internal heat generation. The solution of this differential equation, with a boundary condition,  $T(r_2) = T_2$ , is:

$$T = \frac{\vec{\dot{Q}}_{CEF} - \sum_{j} \vec{\dot{m}}_{j} \left(h_{f,j}^{o} - c_{p,j} T_{ref}\right)}{\sum_{j} \vec{\dot{m}}_{j} c_{p,j}} + \left(T_{2} + \frac{\sum_{j} \vec{\dot{m}}_{j} \left(h_{f,j}^{o} - c_{p,j} T_{ref}\right) - \vec{\dot{Q}}_{CEF}}{\sum_{j} \vec{\dot{m}}_{j} c_{p,j}}\right) \exp\left[\frac{\sum_{j} \vec{\dot{m}}_{j} c_{p,j}}{4\pi k} \left(\frac{1}{r_{2}} - \frac{1}{r}\right)\right]$$
(4)

We can manipulate this equation and receive the following expression for  $\dot{\vec{Q}}_{\scriptscriptstyle CEF}$  :

$$\vec{Q}_{CEF} = \frac{\left(\sum_{j} \vec{m}_{j} h_{f,j} \right|_{r}\right) \exp\left[-\frac{\sum_{j} \vec{m}_{j} c_{p,j}}{4\pi k} \frac{1}{r_{2}}\right] - \left(\sum_{j} \vec{m}_{j} h_{f,j} \right|_{r_{2}}\right) \exp\left[-\frac{\sum_{j} \vec{m}_{j} c_{p,j}}{4\pi k} \frac{1}{r}\right]}{\exp\left[-\frac{\sum_{j} \vec{m}_{j} c_{p,j}}{4\pi k} \frac{1}{r_{2}}\right] - \exp\left[-\frac{\sum_{j} \vec{m}_{j} c_{p,j}}{4\pi k} \frac{1}{r}\right]}$$
(5)

Regarding the thermal resistance definition,  $R = (T_1 - T_2) / \dot{Q}_{1 \to 2}$ , one obtains that the CEF thermal resistance is:

$$\mathbf{R}_{CEF} = \frac{\mathbf{T}_{1} - \mathbf{T}_{2}}{\vec{\mathbf{Q}}_{CEF, 1 \rightarrow 2}} = \frac{\left(\mathbf{T}_{1} - \mathbf{T}_{2}\right) \left( \exp\left[-\frac{\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{c}_{p, j}}{4\pi \mathbf{k} - \mathbf{r}_{2}} \frac{1}{\mathbf{r}_{2}}\right] - \exp\left[-\frac{\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{c}_{p, j}}{4\pi \mathbf{k} - \mathbf{r}_{1}} \frac{1}{\mathbf{r}_{2}}\right] - \left(\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{h}_{f, j}\Big|_{\mathbf{r}_{2}}\right) \exp\left[-\frac{\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{c}_{p, j}}{4\pi \mathbf{k} - \mathbf{r}_{1}} \frac{1}{\mathbf{r}_{2}}\right] - \left(\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{h}_{f, j}\Big|_{\mathbf{r}_{2}}\right) \exp\left[-\frac{\sum_{j} \vec{\mathbf{m}}_{j} \mathbf{c}_{p, j}}{4\pi \mathbf{k} - \mathbf{r}_{1}}\right]$$
(6)

#### 4. A combustion process of a liquid fuel droplet

Combustion phenomena are a significant and extensively studied class of heat transfer problems which involve chemical reactions. Here, we apply the MTRM on a burning liquid fuel droplet, accounting also for a radiation effect. The MTRM is first compared with the classical  $d^2$  model [1], and then radiation is introduced in a simplified manner. Therefore, the present study relies on the same assumptions as those of the classical  $d^2$  model [1] with the addition of assumptions regarding radiation.

The solution of the two models is based on mass conservation, species conservation, liquid-vapor equilibrium, and energy conservation. While the first three principles lead to the same equations, the formulation of the energy conservation equations diverges. Thus, in order to keep the explanation succinct and clear, we present a brief preview of the common final equations and a full analysis of the energy balance equations (illustrated in figure 3).

#### 5. Assumptions

Similarly to the classical  $d^2$  model [1], the present combustion model is based on the following assumptions:

- a) The burning droplet exists in a quiescent, infinite medium, without gravitation influence and with no interactions with adjacent droplets. Thus, the flame around the droplet is spherically symmetric and the problem is one dimensional with radial symmetry.
- b) The chemical kinetics is assumed to be infinitely fast, forming a diffusion flame which can be represented by an infinitesimally thin sheet. In addition, we assume that fuel and oxidizer react at stoichiometric ratio at the flame zone and that all fuel vapors are consumed there.
- c) The fuel is a pure (single-component) liquid with zero solubility for gases; it contains no other components such as soot or water. Phase equilibrium prevails at the liquid-vapor interface.
- d) The gas phase consists of only three "species": fuel vapor, oxidizer, and combustion products. The region outside the flame contains oxidizer and combustion products, whereas the one between the flame and the droplet surface contains fuel vapor and combustion products. Thus, binary diffusion prevails everywhere outside the droplet.
- e) The "onion skin" model is used to describe the liquid core heating/evaporation regime. According to this model, the droplet consists of two zones: an interior one with the initial temperature  $T_0$  and a surface layer at  $T_l$ .
- f) The pressure is uniform and constant.
- g) All thermo-physical properties of the gas components (thermal conductivity, specific heat, and  $\rho D$ ) are uniform (equal for all species), constant, and independent of temperature.
- h) In the explicit solution <u>only</u>, thermal diffusivity and mass diffusivity are assumed to be equal (Lewis number is unity).
- i) The gases behave as ideal gases. They constitute a clear transparent phase, whereas the flame and the droplet behave as gray bodies. In addition, with regard to radiation, the flame is considered as a semitransparent zone with thickness *L*.

#### 5.1 Joint Equations

The continuity equation yields a constant fuel mass flow rate ( $\dot{m}_F$ ) between the droplet and the flame. The simplified combustion model assumes an equal and constant specific heat ( $c_{pg}$ ) with Lewis number of unity for all gaseous species. Thus, one can define:

$$Z = \frac{1}{4\pi\rho\mathcal{D}} = \frac{c_{pg}}{4\pi k_{a}} \tag{7}$$

Where  $\rho$  is the gas density, D is the diffusivity, and  $k_g$  is the thermal conductivity. From species conservation which obeys Fick's law, one obtains two equations:

$$Y_{F,l} = 1 - \exp\left[-Z\dot{m}_F\left(\frac{1}{r_d} - \frac{1}{r_f}\right)\right]$$
(8)

$$\exp\left(\frac{Z\dot{m}_F}{r_f}\right) = \frac{\nu+1}{\nu} \tag{9}$$

where  $Y_{F,l}$  is the fuel mass fraction at the droplet surface,  $\nu$  is the oxidizer to fuel stoichiometric ratio,  $\mathcal{D}$  diffusivity, and  $r_d$  and  $r_f$  the radii of the droplet and the flame, respectively.

The third equation stems from Clausius-Clapeyron equation for the liquid-vapor equilibrium. It yields the following expression for  $Y_{F,l}$  [1]:

$$Y_{F,l} = \frac{A \exp(-B/T_d) M W_F}{A \exp(-B/T_d) M W_F + \left[P - A \exp(-B/T_d)\right] M W_{pr}}$$
(10)

where  $T_d$  is the surface temperature of the droplet.





The energy balance equations for the burning droplet at the flame sheet (F) and the droplet surface (D) are:

F: 
$$\dot{Q}_{cond,f-\infty} - \dot{m}_{ox}h_{ox} + \dot{m}_{pr}h_{pr} + \dot{Q}_{rad,f-\infty} = \dot{m}_{F}h_{F,v} - \dot{Q}_{cond,f-d} - \dot{Q}_{rad,f-d}$$
  
D:  $-\dot{Q}_{rad,f-d} - \dot{Q}_{cond,f-d} + \dot{m}_{F}h_{F,v} = -\dot{Q}_{l} + \dot{m}_{F}h_{F,l}$ 
(11)

where all  $\dot{m}$ 's and  $\dot{Q}$ 's are positive and  $\dot{Q}_{l} = \dot{m}_{F}c_{pl}(T_{d} - T_{i})$ .

In order to express the radiation term between the flame and the droplet, we assume that they behave as two concentric gray spheres, with the following heat transfer rate between them [3]:

$$\dot{Q}_{rad,f-d} = \frac{\sigma 4\pi r_d^2 \left(T_f^4 - T_d^4\right)}{\frac{1}{\varepsilon_d} + \frac{1 - \varepsilon_f}{\varepsilon_f} \left(\frac{r_d}{r_f}\right)^2}$$
(12)

where  $\sigma$  is Stefan-Boltzmann constant, and  $\varepsilon_f$  and  $\varepsilon_d$  are the emissivity of the flame and the droplet, respectively. The formulation of equation system (11) is different for the MTRM and the explicit model. Therefore, a full analysis of each model is shown separately in the following subsections.

# 5.2 MTRM - modified thermal resistance model

The MTRM equalizes between the overall heat flow rates of both sides of each internal heat generation source [1]:

$$\begin{cases} F: & \vec{Q}_{f_{+}} = \vec{Q}_{f_{-}} \\ D: & \vec{Q}_{d_{+}} = \vec{Q}_{d_{-}} \end{cases}$$
(13)

Defining a coupled heat transfer rate for conduction and enthalpy flow, these energy balance equations can be presented as:

$$\begin{cases} F: & \vec{Q}_{CEF,f-\infty} + \vec{Q}_{rad,f-\infty} = \vec{Q}_{CEF,f-d} + \vec{Q}_{rad,f-d} \\ D: & \vec{Q}_{rad,f-d} + \vec{Q}_{CEF,f-d} = -\dot{Q}_l + \dot{m}_F h_{F,l} \end{cases}$$
(14)

or with MTRM formulation as:

$$\begin{cases} F: & \frac{T_{f} - T_{\infty}}{R_{f-\infty}} = \frac{T_{d} - T_{f}}{R_{d-f}} \\ D: & \frac{T_{d} - T_{f}}{R_{d-f}} = -\dot{Q}_{l} + \dot{m}_{F} \left( h_{F,l}^{0} + c_{pl} \left( T_{d} - T_{ref} \right) \right) \end{cases}$$
(15)

where  $R_{f-\infty}$  and  $R_{d-f}$  are the effective thermal resistors between the flame and infinity and the droplet and the flame, respectively. The effective resistors in each region are:

$$\begin{cases} R_{f^{-\infty}} = \frac{1}{\frac{1}{R_{CEF,f^{-\infty}}} + \frac{1}{R_{rad,f^{-\infty}}}} \\ R_{d^{-f}} = \frac{1}{\frac{1}{\frac{1}{R_{CEF,d^{-f}}} + \frac{1}{R_{rad,d^{-f}}}}} \end{cases}$$
(16)

and the thermal resistors for the various heat transfer mechanisms are:

$$\begin{cases} R_{CEF,d-f} = \frac{\left(T_{d} - T_{f}\right) \left[\exp\left(-\frac{Z\dot{m}_{F}}{r_{f}}\right) - \exp\left(-\frac{Z\dot{m}_{F}}{r_{d}}\right)\right] \\ R_{CEF,d-f} = \frac{\left(T_{f} - T_{f}\right) \left(h_{F,v}^{0} + c_{pg}\left(T_{d} - T_{ref}\right)\right) - \dot{m}_{F}\exp\left(-\frac{Z\dot{m}_{F}}{r_{d}}\right) \left(h_{F,v}^{0} + c_{pg}\left(T_{f} - T_{ref}\right)\right) \right) \\ R_{CEF,f-\infty} = \frac{\left(T_{f} - T_{\infty}\right) \left[1 - \exp\left(-\frac{Z\dot{m}_{F}}{r_{f}}\right)\right]}{\dot{m}_{F} \left[ \left(v+1\right) \left(h_{pr}^{0} + c_{pg}\left(T_{f} - T_{ref}\right)\right) - \right] - \dot{m}_{F}\exp\left(-\frac{Z\dot{m}_{F}}{r_{f}}\right) \left[ \left(v+1\right) \left(h_{pr}^{0} + c_{pg}\left(T_{\infty} - T_{ref}\right)\right) - \right] - \dot{m}_{F}\exp\left(-\frac{Z\dot{m}_{F}}{r_{f}}\right) \left[ \left(v+1\right) \left(h_{ox}^{0} + c_{pg}\left(T_{\infty} - T_{ref}\right)\right) - \right] \right] \\ R_{rad,f-d} = \frac{\frac{1}{\varepsilon_{d}} + \frac{1 - \varepsilon_{f}}{\varepsilon_{f}} \left(\frac{r_{d}}{r_{f}}\right)^{2}}{4\pi r_{d}^{2} \sigma \left(T_{f} + T_{d}\right) \left(T_{f}^{2} + T_{d}^{2}\right)} \end{cases}$$

$$(17)$$

# 5.3 Explicit modified d<sup>2</sup> model

The explicit form of equation system (11) is:

$$\begin{cases} F: \qquad -k_g 4\pi r_f^2 \left. \frac{dT}{dr} \right|_{r_{f+}} + k_g 4\pi r_f^2 \left. \frac{dT}{dr} \right|_{r_{f-}} + \frac{\sigma 4\pi r_d^2 \left( T_f^4 - T_d^4 \right)}{\frac{1}{\varepsilon_d} + \frac{1 - \varepsilon_f}{\varepsilon_f} \left( \frac{r_d}{r_f} \right)^2} + \sigma \varepsilon_f 4\pi r_f^2 \left( T_f^4 - T_{\infty}^4 \right) = \dot{m} \Delta h_c \\ D: \qquad \frac{\sigma 4\pi r_d^2 \left( T_f^4 - T_d^4 \right)}{\frac{1}{\varepsilon_d} + \frac{1 - \varepsilon_f}{\varepsilon_f} \left( \frac{r_d}{r_f} \right)^2} + 4\pi r_d^2 k_g \left. \frac{dT}{dr} \right|_{r_{d+}} = \dot{Q}_l + \dot{m} h_{fg} \end{cases}$$
(18)

where  $\Delta h_c = h_{f,F}^o + \nu h_{f,ox}^o - (1+\nu) h_{f,pr}^o$  and  $h_{fg} = h_v - h_l$ .

From the one dimensional Shvab-Zeldovich energy equation (Turns [1], p. 245), one obtains the temperature profile and its derivative in the gaseous zones between the droplet and the flame (d-f), and between the flame and infinity ( $f-\infty$ ):

d-f:  

$$\begin{cases}
T(r) = \frac{\left(T_d - T_f\right) \exp\left(\frac{-Z\dot{m}_F}{r}\right) + T_f \exp\left(\frac{-Z\dot{m}_F}{r_d}\right) - T_d \exp\left(\frac{-Z\dot{m}_F}{r_f}\right)}{\exp\left(-\frac{Z\dot{m}_F}{r_d}\right) - \exp\left(-\frac{Z\dot{m}_F}{r_f}\right)} \\
\frac{dT}{dr} = \frac{Z\dot{m}_F}{r^2} \frac{\left(T_d - T_f\right)}{\exp\left(-\frac{Z\dot{m}_F}{r_d}\right) - \exp\left(-\frac{Z\dot{m}_F}{r_f}\right)} \exp\left(-\frac{Z\dot{m}_F}{r_f}\right)
\end{cases}$$
(19)

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$$f^{-\infty}: \begin{cases} T(r) = \frac{\left(T_f - T_{\infty}\right) \exp\left(\frac{-Z\dot{m}_F}{r}\right) + T_{\infty} \exp\left(\frac{-Z\dot{m}_F}{r_f}\right) - T_f}{\exp\left(-\frac{Z_T\dot{m}_F}{r_f}\right) - 1} \\ \frac{dT}{dr} = \frac{Z\dot{m}}{r^2} \frac{\left(T_f - T_{\infty}\right)}{\exp\left(-\frac{Z\dot{m}_F}{r_f}\right) - 1} \exp\left(\frac{-Z\dot{m}_F}{r}\right) \end{cases}$$
(20)

Substituting equations (19) and (20) into equation system (18), one obtains:

$$\begin{cases} F: \qquad c_{pg}\dot{m}_{F}\nu\left(T_{f}-T_{\infty}\right)+\frac{c_{pg}\dot{m}_{F}\left(T_{d}-T_{f}\right)}{\exp\left[-Z\dot{m}_{F}\left(\frac{1}{r_{d}}-\frac{1}{r_{f}}\right)\right]-1}+\frac{\sigma 4\pi r_{d}^{2}\left(T_{f}^{4}-T_{d}^{4}\right)}{\frac{1}{\varepsilon_{d}}+\frac{1-\varepsilon_{f}}{\varepsilon_{f}}\left(\frac{r_{d}}{r_{f}}\right)^{2}}+\sigma \varepsilon_{f} 4\pi r_{f}^{2}\left(T_{f}^{4}-T_{\infty}^{4}\right)=\dot{m}\Delta h_{c} \\ \\ D: \qquad \frac{\sigma 4\pi r_{d}^{2}\left(T_{f}^{4}-T_{d}^{4}\right)}{\frac{1}{\varepsilon_{f}}+\frac{1-\varepsilon_{f}}{\varepsilon_{f}}\left(\frac{r_{d}}{r_{f}}\right)^{2}}+\frac{c_{pg}\dot{m}_{F}\left(T_{d}-T_{f}\right)}{1-\exp\left[-Z\dot{m}_{F}\left(\frac{1}{r_{f}}-\frac{1}{r_{d}}\right)\right]}=\dot{Q}_{l}+\dot{m}h_{fg} \end{cases}$$
(21)

#### **5.4 Solution summary**

Both models converge into five equations whose solution predicts the five combustion characteristics:  $r_f$ ,  $T_f$ ,  $T_d$ ,  $Y_{F,I}$ , and  $\dot{m}_F$ . One may show that mathematically equation system (15) of the thermal resistance model is identical to equation system (21) of the classical model, resulting with the same solutions, as obtained numerically (in the next Section).

#### 5.5 Results for a burning n-heptane droplet

To validate the model and demonstrate its application, a complete combustion process of a 1-mm radius n-heptane droplet dyed with soot has been simulated. Both the classical combustion model and the thermal resistance model were applied in each iteration to predict the combustion characteristics  $r_f$ ,  $T_f$ ,  $T_d$ ,  $Y_{F,l}$ , and  $\dot{m}_F$ , using the data as explained

below and appear in the appendix.

We assume the dyed droplet to be opaque with emissivity of ~0.9. The emissivity of the flame is described by Bouguer-Beer law for a semi-transparent, non-reflecting medium:

$$\varepsilon_f = \alpha_f = 1 - \exp(-\kappa_p L) \tag{22}$$

where L is the path way and  $\kappa_p$  is the Planck mean absorption coefficient (in units of m<sup>-1</sup>), expressed as [3, 5]:

$$\kappa_p = \sum_i \kappa_{g,i} + \kappa_s = \kappa_{CO_2} + \kappa_{H_2O} + \kappa_s \tag{23}$$

The Planck mean absorption coefficient of the soot in units of m-1 is equal to [6]:

$$\kappa_s = 2263 f_v T \tag{24}$$

where  $f_{\nu}$  is the soot fraction and  $\kappa_s$  is given in units of m<sup>-1</sup>. The Planck mean absorption coefficient of CO<sub>2</sub> and H<sub>2</sub>O is given by [7]:

$$\kappa_{g,i} = c_0 + c_1 \frac{1000}{T} + c_2 \left(\frac{1000}{T}\right)^2 + c_3 \left(\frac{1000}{T}\right)^3 + c_4 \left(\frac{1000}{T}\right)^4 + c_5 \left(\frac{1000}{T}\right)^5$$
(25)

in units of m<sup>-1</sup>atm<sup>-1</sup>, with the following coefficients (Table 1):

Table 1: The Polynomial coefficients of the Planck mean absorption coefficients of CO<sub>2</sub> and H<sub>2</sub>O

Ι	$H_2O$	$CO_2$
$C_0$	-0.23093	18.741
$C_1$	-1.1239	-121.31
$C_2$	9.4153	273.5
$C_3$	-2.9988	-194.05
$C_4$	0.51382	56.31
C5	-1.868.10-5	-5.8169

In order to obtain  $\kappa_g$  in units of m<sup>-1</sup>, it has to be multiplied by the partial pressures of the absorbing species; in our case 0.169P for CO<sub>2</sub> and 0.193P for H<sub>2</sub>O.

Figures 4-6 present the predicted droplet surface temperature, flame temperature, and fuel vapor mass flow rate, respectively, vs. the droplet radius, as the combustion process proceeds, starting from a 1-mm-radius droplet. The calculations were made for cases with and without radiation effect. As mentioned, the results of both the classical formulation (as presented in Ref. [4]) and the current thermal resistance model (MTRM) are identical.



Figure 4: a) The surface temperature of a 1-mm-radius burning droplet vs. the instantaneous droplet radius for two cases – with and without radiation. b) The fuel vapor mass fraction at the droplet surface vs. the droplet radius.

The surface temperature and the fuel vapor mass fraction at the droplet surface are correlated as expected (from Clausius-Clapeyron equation). Their values remain relatively constant during most of the burning process, except at the end when the droplet is very small. The radiation depends on the radius of the droplet. As the radius decreases, its influence and the heat transferred to the droplet reduce, leading to a decrease in the temperature of the droplet surface.



Figure 5: The flame temperature vs. the droplet radius.

In addition, the radiation couples between the flame temperature and that of the droplet surface. Thus, as the droplet shrinks, the flame temperature increases.



Figure 6: a) The flame radius vs. the droplet radius. b) The fuel vapor mass flow rate vs. the droplet radius.

The flame radius and the fuel mass flow rate decrease linearly with the radius of the droplet. Furthermore, a correlation prevails between the two graphs, probably since higher mass flow rate of the vapors pushes the flame outward. In addition, the linear trend of the mass flow rate (which is proportional to  $r^2$ ) implies the expected result of the  $d^2$  model. However, at small radii (smaller than 0.1 mm), the trend of the graph with the radiation deviates and coincides with the one which does not consider the radiation. This may stem from the negligible effect of the radiation at small radii.

It may be mentioned that our approximated model assumes that the flame and the droplet behave as grey bodies (with a semi-transparent medium) and emissivity for average temperature. The emissivity values and these assumptions might be inaccurate and lead to overestimation of the radiation. However, radiation was considered in order to demonstrate the use and the advantages of the MTRM over the explicit model (and not to accurately predict the behavior of the droplet).

# 6. Conclusions

The modified thermal resistance model (MTRM) was applied to solve a combustion process of a liquid fuel droplet. The results were compared to those of the classical  $d^2$  model and an absolute correlation was obtained. This case exhibits the use of the MTRM and may stimulate the reader mind about further possible applications.

The MTRM reliance on only few assumptions makes it a modular and very robust technique. Furthermore, its simple formulation allows the user to solve complex cases relatively fast and to easily regard multiple heat transfer mechanisms. The MTRM does not require a deep understanding of the problem, but only knowing the heat transfer mechanisms involved.

In addition, the MTRM may help improve some combustion models. For example, one may achieve a more accurate result by dividing the space into a number of regions with constant properties within each region. In other case, one can treat the flame sheet as a flame "zone", equivalent to multiple flame sheets with partial reaction at each sheet. Nonetheless, it requires a-priori knowledge of the chemical reaction zone thickness.

In conclusion, the MTRM is a powerful novel technique. It can help solving various one-dimensional quasi-steady heat transfer problems that includes chemical reactions.

# Appendix

Table 2 summarizes the values of parameters used in the solution of the combustion of n-heptane. All thermo-physical properties were taken from the books of Turns [1] and Incorpera [4] (except fv and L which were taken from Ref. 3). The thermo-physical properties of the gas are given at the average temperature between the flame and the liquid fuel. Because of the large difference in the flame temperature between the two cases, with and without radiation, two average temperatures were used, according to the case.

Parameter	Value	
ν	15.07 kg/kg	
A	28386 atm	
В	3808 K	
$MW_F$	100 kg/kmol	
$MW_{pr}$	28.56 kg/kmol	
Р	1 atm	
T <sub>b</sub>	371.42 K	
$T_{\infty}$	300 K	
$\overline{\mathrm{T}}$	1035 K (with radiation)	
	1435 K (without radiation)	
ρι	684 kg/m <sup>3</sup> (at 300K)	
$c_{pg}$	1147 J/kg K (air at 1035K)	
	1215 J/kg K (air at 1435K)	
$c_{pl}$	1897 J/kg K (at 350K)	
$k_{g}$	0.0684 W/m K (at 1035K)	
	0.0941 W/m K (at 1435K)	

Table 2: Summary of the parameter values used in the solution of n-heptane droplet combustion

r <sub>d</sub>	10 <sup>-3</sup> m	
σ	$5.67{\cdot}10^{-8}~W/m^2~K^4$	
$rac{arepsilon_{ m d}}{{ m f}_{ m v}} \ L \ h_{fg}$	0.9 ~10 <sup>-6</sup> 3·10 <sup>-3</sup> m 316 kJ/kg	
$\Delta h_c$	44.93 MJ/kg	
$h^0_{f,F,l}  onumber \ h^0_{f,F,v}$	1.878 MJ/kg -1.562 MJ/kg	
$h_{f,ox}^0$	0 J/kg	
$h_{f,pr}^0$	-2.893 MJ/kg	
$T_i$	300 K	

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