# SHVAB-ZEL'DOVICH AND FLAMELET FORMULATIONS APPLIED ON QUASI-STEADY DROPLET COMBUSTION WITH SOOT FORMATION AND RADIATIVE HEAT TRANSFER

Lucas Soares Pereira

Scientific Initiation Report of the program PIBIC, advised by Dr. Fernando Fachini Filho.

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INPE
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**ABSTRACT**

The present work, that started in August 2019, studies theoretically the quasi-steady combustion of an isolated droplet with the formation of soot. For this, an analysis was made on the conservation equations to determine the characteristic spatial and temporal scales of the problem, which were used for the nondimensionalization of those equation. The problem has spherical symmetry, which allows for a one-dimensional analysis of the problem. The quasi-steady combustion regime is justified by the fact that the thermal inertia of the gas phase close to the droplet is much less than that of the liquid phase, so the environment adapts thermically much faster than the droplet. The boiling temperature is considered for the whole droplet, i.e., all heat transferred to the droplet is used for the phase change (vaporization). It was admitted that the chemical process occurs at the Burke-Schumann limit, thus the reaction rate is infinitely fast which leads to infinitely thin flame. To solve the system of governing differential equations, the Shvab-Zel'dovich formulation was used, which eliminates the dependence of the chemical reaction term, which is non-linear. Therefore, the mass fraction of species and the temperature field are described by the mixture fraction, Z, and excess enthalpy, H, equations. The boundary conditions were imposed at the surface of the droplet and in a region far from it. To describe the formation of soot in the problem, a simplified mathematical model was adopted. The resulting system of second order differential equations allow to be integrated analytically once, and the final system of first order differential equations is integrated numerically. The transport properties were considered as constant, the that allowed us to find analytical solutions for the system of differential equations resulting. The next step will be to implement a computational code to solve the system of nonlinear algebraic equations.

Keywords: Droplet combustion. Shvab-Zel'dovich. Soot Formation.

# FORMULAÇÕES DE SHVAB-ZEL´DOVICH E FLAMELET APLICADAS À COMBUSTÃO QUASE ESTÁVEL DE GOTÍCULA, COM FORMAÇÃO DE FULIGEM E TRANSFERÊNCIA RADIATIVA DE CALOR

## RESUMO

O presente trabalho, que foi iniciado em Agosto de 2019, estuda teoricamente a combustão no regime quase-estacionário de uma gota isolada com a formação de fuligem. Para isso, foi feita uma análise das equações de conservação para determinar as escalas espaciais e temporais características do problema, as quais foram utilizadas para a adimensionalização dessas equações. O problema tem simetria esférica, o que permite uma análise unidimensional. O regime de combustão quase-estacionário é justificado pelo fato de que a inércia térmica da fase gasosa próxima à gota é muito menor que a da fase líquida, de modo que o ambiente se adapta muito mais rapidamente que a gota. A temperatura de ebulição foi considerada para toda a gota, isto é, todo o calor transferido para ela é usado para a mudança de fase (vaporização). Foi admitido que o processo químico ocorre no limite de Burke-Schumann, portanto a taxa de reação é infinitamente rápida, o que leva a chamas infinitamente finas. Para resolver o sistema de equações diferenciais governantes, foi utilizada a formulação de Shvab-Zeldovich, que elimina a dependência do termo de reação química, que não é linear. Portanto, a fração de massa das espécies e o campo de temperatura são descritos pelas equações da fração da mistura, Z, e de excesso de entalpia, H. As condições de contorno foram impostas na superfície da gota e em uma região distante da mesma. Para descrever a formação de fuligem no problema, foi adotado um modelo matemático simplificado. O sistema resultante de equações diferenciais de segunda ordem permite uma integração analítica, e o sistema final de equações diferenciais de primeira ordem é integrado numericamente. As propriedades de transporte foram consideradas como constantes, o que permitiu encontrar soluções analíticas para o sistema de equações diferenciais resultante. O próximo passo será implementar um código computacional para resolver o sistema de equações algébricas não lineares.

Palavras-chave: Combustão de gotícula. Shvab-Zel'dovich. Formação de fuligem.

# LIST OF FIGURES

# LIST OF ABBREVIATIONS

CNPq  –  Conselho Nacional de Desenvolvimento Científico e Tecnológico
INPE  –  Instituto Nacional de Pesquisas Espaciais

# LIST OF SYMBOLS

| | | |
|---|---|---|
| t | – | Time |
| a | – | Radius of droplet |
| L | – | Latent Heat |
| k | – | Thermal Conductivity |
| T | – | Temperature |
| r | – | Radial coordinate |
| $a_0$ | – | Initial droplet radius |
| $c_p$ | – | Specific heat at constant pressure |
| p | – | Pressure |
| $\mathbf{I}$ | – | Identity matrix |
| $\mathbf{S}$ | – | Viscous stress tensor |
| V | – | Volume |
| $\mathbf{v}$ | – | Velocity vector |
| $\mathbf{n}$ | – | Normal vector |
| $D_i$ | – | Mass diffusivity |
| $Y_i$ | – | Mass fraction |
| $s_i$ | – | Stoichiometric Coefficient |
| B | – | Frequency factor |
| E | – | Activation Energy |
| R | – | Gas constant |
| $\mathbf{f}$ | – | Field force vector |
| U | – | Total energy |
| $\dot{W}$ | – | Work production rate |
| $\dot{Q}$ | – | Heat transfer rate |
| $\mathbf{q}$ | – | Heat flux |
| e | – | Internal energy |
| h | – | Enthalpy |
| Q | – | Combustion heat |
| $\dot{m}$ | – | Dimensional vaporisation rate |
| v | – | Dimensionless radial velocity |
| $Le_i$ | – | Lewis number of specie i |
| Da | – | Damköhler number |
| x | – | Nondimensional radial coordinate |
| $T_B$ | – | Boiling Temperature |
| $T_f$ | – | Flame temperature |
| $y_{Fs}$ | – | Mass fraction of fuel in surface of droplet |
| Z | – | Mixture fraction |
| H | – | Excess enthalpy |
| $Q_{soot}$ | – | Heat to form a unit mass of soot |
| $x_{soot}$ | – | Position of the soot formation |
| $T_s$ | – | Surface Temperature |
| $\rho$ | – | Density |
| $\alpha$ | – | Thermal diffusivity |

| | | |
|---|---|---|
| $\tau$ | – | Contact force tensor |
| $\omega$ | – | Chemical reaction term |
| $\nu$ | – | Cinematic Viscosity |
| $\mu$ | – | Dynamic Viscosity |
| $\lambda$ | – | Nondimensional vaporisation rate |
| $\dot{\omega}$ | – | Dimensionless chemical reaction term |
| $\dot{\omega}_{soot}$ | – | Nondimensional chemical reaction term for soot |
| $\phi_m$ | – | Mass of soot |
| $\phi_q$ | – | Heat required for soot formation |

# CONTENTS

# 1 INTRODUCTION

The oldest technology of the human species is combustion (WARNATZ et al., 2006). Following the timeline of our species, we note that combustion is present in the main historical moments in which there was a scientific and technological leap, enabling greater development of our society in each era. Three important periods where combustion was the central theme were the Industrial Revolutions in the 18th and 19th centuries, and during the 20th century. The discoveries of each era allowed some developments such as steam engines, internal combustion engines, aerospace and energy sector developments, where mathematics, chemistry and physics, played a fundamental role in the description of the phenomena (DALENOGARE, 2017; BIANCHIN, 2016).

Combustion consists of the chemical reaction involving the fuel and the oxidizer, where there are breaks in the chemical bonds of each reagent and the formation of combustion products, in addition to the release of energy in the form of heat and light. This reaction can occur quickly or slowly, with direct implications for the release of heat and light emission (TURNS, 2011). In the combustion reaction, soot formation can occur, which is generated by the unburned fuel in the flame. Soot contributes to damage the environment, such as acid rain and rising temperatures on the planet, in addition, it compromises structural projects, such as the accumulation of soot on the walls of a combustor. On the other hand, soot particles can contribute to industrial ovens, for example, where the thermal radiation transferred during combustion can be used (MERGULHÃO, 2016).

In order to optimize the burning of the fuel, it is atomized, where the liquid phase breaks down into small droplets. This process aims to increase the contact area between the fuel and the ambient atmosphere, resulting in an increase in the rate of heat transfer from the environment to the fuel and increasing the rate of vaporization. Analyzing the heat and mass transfer in a droplet cloud is a highly complex process, so an isolated droplet study is done, and it contributes to the description of the droplet cloud behavior (DALENOGARE, 2017)

In this work, which was funded and supported by CNPq and INPE, an analysis of temporal and spatial scales is carried out. In addition, we deduce the conservation equations, which form the basis for solving the problem. The equations were written in their dimensionless form, taking into account the characteristic scales, which allowed the simplification of the equations according to the physical conditions of the combustion of an isolated droplet. Besides, from detailed equations for conservation

of mass, species and energy for the liquid and gaseous phases, a mathematical description of the combustion of an isolated droplet, of spherical symmetry, inserted in an oxidant, quiescent ambient atmosphere, is presented. Due to the presence of a strongly nonlinear term in the species and energy conservation equations, the Shvab-Zel'dovich formulation is adopted to combine the equations and eliminate the chemical reaction term. Only soot formation is considered in the mathematical formulation, heat transfer is added in the next works.

## 2 DESCRIPTION OF THE PROBLEM AND SCALES

The objective of this work is to study the combustion of a droplet of liquid fuel inserted in an oxidant ambient atmosphere with soot formation, using the Shvab-Zel'dovich formulation. No relative velocity between the droplet and the environment is considered, thus the convective effects on the vaporization is neglected. Also the vaporization process generates a low velocity and only in radial direction, the viscous dissipation is zero. Due to the fact that the size of droplets in industrial and aerospace application are very small, the gravity effects can be disregarded.

For combustion to occur, fuel and oxidant must be in the gaseous phase, thus the burning of a fuel droplet demands its vaporization. It is assumed that the droplet temperature is uniform and equal to the boiling temperature. Therefore, heat transferred from the ambient atmosphere is used to vaporize the liquid phase. Since there is no relative velocity between droplet and environment, then the velocity inside the droplet is zero. Therefore the droplet presents spherical symmetry, and the problem is described by 1D conservation equations.

The liquid fuel evaporates and diffuses to the reaction zone. The expansion of the gaseous phase, which is caused by the phase change and the increasing temperature toward the flame, has a much smaller velocity than the speed of sound, which explains the constant pressure.The stoichiometric ratio between fuel and oxidant fluxes is the necessary condition to define the location of the reaction zone, where a spherically symmetrical flame is established. At the flame heat is generated and transferred to the droplet to provide the vaporization. Let's consider that the gas phase is in a low pressure condition, justifying the quasi steady regime. The reason for that is the higher thermal inertia of the liquid phase than that of the gas phase. Therefore, the gas phase adapts quickly to temperature variation on the droplet surface. This characteristic of the problem simplifies the conservation equations, eliminating the need to deal with the time evolution of the temperature inside the droplet.

We consider that the combustion occurs at the Burke-Schumann limit, that is, the number of Damkohler is infinitely large, so the chemical reaction time must be infinitely greater than any mechanical time. This makes the residence time of the reagents infinitely short in the reaction zone, which generates an infinitely narrow flame. Under this condition, the domain can be divided in fuel zone and oxygen zone, and the integration of the conservation equations can be performed in a easy way. The temperature of the gas phase varies with distance, assuming greater value

in the position of the flame, in which the mass fraction of fuel and oxidant goes to zero.

The problem of combustion of an isolated droplet involves transfer of mass by diffusion, transfer of energy, in addition to the generation and consumption of chemical species. The properties of the gas, in the environment far from the droplet, are constant. These properties are: density $\rho_\infty^*$, thermal conductivity $k_\infty^*$, constant pressure specific heat $c_P^*$. The gas temperature and the mass fraction of the oxidant are kept constant at $T_\infty^*$ and $Y_{O\infty}^*$.

In this work, the superscript "*" indicates the variable in dimensional form and the subscript $\infty$ and b indicates the ambient condition (far from droplet) and boiling condition, respectively.

## 2.1 Soot Formation

Ideally, the combustion of hydrocarbons has mainly the formation of carbon dioxide and water, as shown in the equation below.

$$C_xH_y + (x + y/4)O_2 \rightarrow xCO_2 + y/2H_2O \tag{2.1}$$
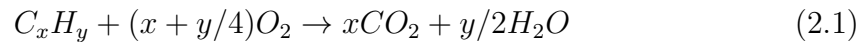
An ideal condition means that the oxygen content of the mixture is sufficient to react with all the fuel. In practice, the conditions are different from the ideal, that is, if the oxygen present is not sufficient to fully convert the fuel according to Eq. (2.1), and if the fuel pyrolysis to occur, the formation of other combustion products besides carbon dioxide and water, such as carbon monoxide, hydrogen, hydrocarbons and soot are observed.

Soot formation is a process that converts a hydrocarbon fuel molecule containing few carbon atoms into an agglomerated carbonaceous, which has a few million carbon atoms. This step is described by the formation and growth of large aromatic hydrocarbons and their transition to particles, after which comes the coagulation of the primary particles, forming even larger aggregates, and, finally, the growth of solid particles (BOCKHORN, 1994). Soot forms around the droplet. Its geometric shape has the shape of a ring or a shell. This ring, formed by an aggregate of soot, is reasonably dense, but highly porous. The position of the sooty shell is determined by balancing the thermophoretic and drag forces (KUMAR et al., 2002)

Figure 2.1 shows the position of the droplet, the soot shell and the flame. The region outside the flame represents the gaseous and oxidizing atmosphere.

Figure 2.1 - Schematic of problem configuration showing the liquid-fuel droplet, flame zone, soot layer, and the associated forces.

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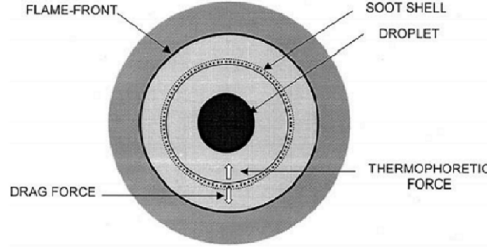
In this work, an infinitely fast reaction is considered, then the soot particles are formed only by the pyrolysis of fuel in the region of temperature around $1200K$, given by a first order reaction $F \rightarrow Soot$. The term of chemical kinetics related with the soot formation is modelled in simple form as

$$\hat{\dot{\omega}}_{soot} = \lambda_{soot}\delta(x - x_{soot})$$

in which $\lambda_{soot}$ is the amount of soot generated, $\delta(x - x_{soot})$ is the delta of Dirac and $x_{soot}$ is the position of the soot formation (FACHINI, 2006).

## 2.2 Scales

In order to study physical phenomena, it is extremely important to have a characteristic parameter in order to be able to classify how different things are. These parameters are the length, time and velocity scales. In this work, all lengths are scaled with initial droplet radius.

The droplet has a time to evaporate. This time can be calculated due to the fact that all heat conducted to the droplet is equal to the energy required to evaporate

the liquid fuel (GOLDSMITH, 1955), thus

$$\frac{d}{dt^*}\left(\frac{4}{3}\pi(a^*)^3\rho_l^*L^*\right) = 4\pi(a^*)^2 k_\infty^* \left.\frac{dT^*}{dr^*}\right|_a$$

$$4\pi\rho_l^*L^*(a^*)^2\frac{\Delta a^*}{\Delta t^*} \sim 4\pi(a^*)^2 k_\infty^*\frac{\Delta T^*}{\Delta r^*}$$

$$\rho_l^*L^*\frac{-a_0^*}{t_{vap}^*} = k_\infty^*\frac{T_\infty^* - Tb}{-a_0^*}$$

$$t_{vap}^* = \frac{\rho_l^*(a_0^*)^2}{k_\infty^*}\frac{L^*}{T_\infty^* - T_b^*}$$

$$t_{vap}^* = \frac{\rho_l^*}{\rho_\infty^*}\frac{\rho_\infty^* c_p^*(a_0^*)^2}{k_\infty^*}\frac{L^*}{c_p^*(T_\infty^* - T_b^*)}$$

$$t_{vap}^* = \frac{\rho_l^*}{\rho_\infty^*}\frac{(a_0^*)^2}{k_\infty^*/(c_p^*\rho_\infty^*)}\frac{L^*}{c_p^*(T_\infty^* - T_b^*)}$$

In which

$$\frac{L^*}{c_p^*(T_\infty^* - T_b^*)}$$

have a order of unit and

$$\epsilon = \frac{\rho_\infty^*}{\rho_l^*} \qquad \alpha_\infty^* = \frac{k_\infty}{c_p^*\rho_\infty^*}$$

Therefore, the characteristic time is given by the vaporization time of the droplet

$$t_{vap}^* = \frac{(a_0^*)^2}{\alpha_\infty^*\epsilon}$$

Since the droplet is at the boiling temperature, so there is no need to consider heating the droplet.

## 3 MATHEMATICAL MODEL

In this mathematical description, the main topics studied were based on the texts of (GUIDORIZZI, 2002; FACHINI, 1999; FOX et al., 2014; BIANCHIN, 2016; DALENOGARE, 2017).

First of all, are presented the conservation equations in the gas and liquid in dimensional form. To describe this formulation we applied the Reynolds Transport Theorem, Gauss Theorem and physics laws such as Second Newton's Law and First Thermodynamics Law, and mass conservation. In this work, we adopted the global one-step mechanism to describe the combustion reaction, which is represented as follows

$$F + sO_2 \rightarrow (1 + s)P \tag{3.1}$$

The Reynolds Transport Theorem establishes the relationship between the variation of a system property and the formulation of the control volume,

$$\frac{d}{dt} \int_{V_f} \phi(\mathbf{x}, t) dV = \int_{V_c} \frac{\partial \phi(\mathbf{x}, t)}{\partial t} dV + \int_{\Sigma_c} \phi(\mathbf{x}, t) \mathbf{v} \cdot \mathbf{n} dA$$

in which $V_f$ is fluid volume, or system volume, $V_c$ is control volume and $\Sigma_c$ is the surface of control volume.

Gauss Theorem or Divergence Theorem establishes the following relationship

$$\int_V \nabla \cdot \mathbf{F} dV = \int_\Sigma \mathbf{F} \cdot \mathbf{n} dA$$

in which V is the volume of a region, $\Sigma$ is the boundary surface of V and $\mathbf{n}$ is the normal vector of the surface and is positively oriented, that is, out of the region. $\mathbf{F}$ is a vector field whose components have continuous partial derivatives in the region containing V.

The surface forces can be write as following

$$\tau^* = -p^* \mathbf{I}^* + \mathbf{S}^*$$

For liquid phase is considered $\rho_l$ constant, the velocity between gas phase and liquid phase is zero, pressure is constant and the reaction term is disregarded because $Y_O = 0$ inside the droplet.

### 3.1 Conservation Equations for the Gas Phase

#### 3.1.1 Mass Conservation

In the control volume there is no creating or destroying of mass, therefore

$$\frac{d}{dt^*} \int_{V_f} \rho^* dV^* = 0$$

Applying the Reynolds Transport Theorem

$$\int_{V_c(t)} \frac{\partial \rho^*}{\partial t^*} dV^* + \int_{\Sigma_c(t)} \rho^* \mathbf{v}^* \cdot \mathbf{n}^* dA^* = 0$$

where

$$\int_{\Sigma_c(t)} \rho^* \mathbf{v}^* \cdot \mathbf{n}^* dA^* = \int_{V_c(t)} \nabla \cdot \rho^* \mathbf{v}^* dV^*$$

satisfies the Gauss Theorem. Therefore, the Mass Conservation Equation is

$$\frac{\partial \rho^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* = 0 \tag{3.2}$$

The process to find conservation equations is repetitive, that is, we will always use the previous step.

#### 3.1.2 Species Conservation

The rate of change in the mass of species i is related to the diffusion of that species across the control surfaces and the rate of chemical reaction, which can create or destroy the species. Mathematically

$$\frac{d}{dt} \int_{V_f(t)} \rho_i^* dV^* = \int_{\Sigma_c(t)} -\rho^* D_i^* \nabla Y_i^* \mathbf{n}^* dA^* + \int_{V_c(t)} s_i \rho^* \omega^* dV^*$$

in which $s_F = 1$, $s_O = s$, according to Eq. (3.1),

$$Y_i^* = \frac{\rho_i^*}{\rho^*} \qquad \omega^* = B Y_F^* Y_O^* e^{-E^*/(R^* T^*)}$$

Applying the Reynolds Transport Theorem and Gauss Theorem we have the Species Conservation Equation

$$\frac{\partial \rho^* Y_i^*}{\partial t^*} + \nabla \cdot \rho^* Y_i^* \mathbf{v}^* = -\nabla \cdot \rho^* D_i^* \nabla Y_i^* + s_i \rho^* \omega^* \tag{3.3}$$

8

### 3.1.3 Momentum Conservation

The second Newton's law describe the relation between the rate of change of momentum of a body and the forces applied to it. The forces applied to the fluid are contact forces

$$\int_{\Sigma_f(t)} \tau^* \cdot \mathbf{n}^* dA^*$$

and field forces

$$\sum_k \int_{V_f}^* \rho^* \mathbf{f}_k^* dV^*$$

Analyzing the forces in the fluid and applying the Reynolds Transport Theorem and Gauss Theorem, we have

$$\frac{\partial \rho^* \mathbf{v}^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* \mathbf{v}^* = \nabla \cdot \tau^* + \sum_k \rho^* \mathbf{f}_k^* \tag{3.4}$$

We can obtain the equation for the conservation of kinetic energy by multiplying Eq. (3.4) in non-conservative form by $\mathbf{v}$:

$$\frac{\partial}{\partial t^*}(\rho^* \frac{(v^*)^2}{2}) + \nabla \cdot \left( \rho^* \mathbf{v}^* \frac{(v^*)^2}{2} \right) = \mathbf{v}^* \cdot \nabla \cdot \tau^* + \sum_k \rho^* \mathbf{v}^* \cdot \mathbf{f}_k^* \tag{3.5}$$

### 3.1.4 Energy Conservation

To describe the energy conservation we must analyze the First Law of Thermodynamics

$$\Delta U^* = Q^* + W^*$$

The rate of change in total energy is equal to the change in work and heat per unit time.

$$\frac{d}{dt} \int_{V_f(t)} \rho^* U^* dV^* = \dot{W}^* + \dot{Q}^*$$

in which the change of work per unit time is equal to the change of volumetric and surface forces, and the change of heat per unit time is equal to the heat flows through the control surface and the heat generation inside the control volume. Thus

$$\frac{d}{dt} \int_{V_f(t)} \rho^* U^* dV^* = \int_{V_f} \nabla \cdot (\mathbf{v}^* \cdot \tau^*) dV^* + \int_{V_c(t)} \sum_k \rho^* \mathbf{v}^* \cdot \mathbf{f_k}^* dV^* + \int_{\Sigma_c(t)} \mathbf{q}^* \cdot \mathbf{n}^* dA^*$$

Therefore, the Total Energy Conservation Equation is

$$\frac{\partial}{\partial t}\rho^* U^* + \nabla \cdot \left( \rho^* \mathbf{v}^* U^* \right) - \nabla \cdot (\mathbf{v}^* \cdot \tau^*) - \sum_k \rho^* \mathbf{v}^* \cdot \mathbf{f}_k^* + \nabla \cdot \mathbf{q}^* = 0 \tag{3.6}$$

9

in which

$$U^* = e^* + \frac{1}{2}(v^*)^2$$

The internal energy is the difference

$$e^* = U^* - \frac{1}{2}(v^*)^2$$

Therefore, the internal energy equation is obtained by subtracting the Eq.(3.4) from Eq.(3.5)

$$\frac{\partial \rho^* e^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* e^* = -p^* \nabla \cdot \mathbf{v}^* + \nabla \mathbf{v}^* : \mathbf{S}^* + \nabla \cdot k^* \nabla T^* + \nabla \cdot \sum_k (\rho^* D_k^* \nabla Y_k^* h_k^*) \quad (3.7)$$

in which

$$\mathbf{q}^* = k^* \nabla T^* - \sum_k (\rho^* D_k^* \nabla Y_k^*) h_k^*$$

$$\nabla \cdot (\mathbf{v}^* \cdot \mathbf{S}^*) = \mathbf{v}^* \cdot \nabla \cdot \mathbf{S}^* + \nabla \mathbf{v}^* : \mathbf{S}^*$$

$$-\nabla \cdot \mathbf{v}^* p^* = -p^* \nabla \cdot \mathbf{v}^* - \mathbf{v}^* \nabla p^*$$

### 3.1.5 Enthalpy Conservation

Here, we substitute $e^* = h^* - p^*/\rho^*$ in Eq.(3.6) and expand the left hand side to get

$$\frac{\partial \rho^* h^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* h^* = \frac{\partial p^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla p^* + \nabla \mathbf{v}^* : \mathbf{S}^* + \nabla \cdot k^* \nabla T^* + \nabla \cdot \sum_k (\rho^* D_k^* \nabla Y_k^*) h_k^*$$

Total enthalpy is the sum of the variation of sensitive enthalpy $((h^*)^T)$ and enthalpy of formation $((h_k^*)^0)$

$$h^* = \sum_k [Y_k^* (h_k^*)^0 + (h_k^*)^T] = Y_k^* (\bar{h_k^*})^0 + \bar{h}^*$$

$$Y_k^* \bar{h}^{*0}_k = \sum_k Y_k^* (h_k^*)^0$$

$$\bar{h}^* = \sum_k Y_k^* (h_k^*)^T$$

Making the substitutions, we arrive at the enthalpy conservation equation

$$\frac{\partial \rho^* \bar{h}^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* \bar{h}^* - \nabla \cdot \sum_k (\rho^* D_k^* \nabla Y_k^*)(h_k^*)^T = \frac{\partial p^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla p^* + \nabla \mathbf{v}^* : \mathbf{S}^* + Q^* \omega^* + \nabla \cdot k^* \nabla T^*$$

The term of heat transfer by mass diffusion

$$\nabla \cdot \sum_k (\rho^* D_k^* \nabla Y_k^*)(h_k^*)^T$$

is only relevant when the species present great differences in their molecular masses. In this work this phenomenon can be disregarded. Finally

$$\frac{\partial \rho^* \bar{h}^*}{\partial t^*} + \nabla \cdot \rho^* \mathbf{v}^* \bar{h}^* = \frac{\partial p^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla p^* + \nabla \mathbf{v}^* : \mathbf{S}^* + \nabla \cdot k^* \nabla T^* + Q^* \omega^* \qquad (3.8)$$

## 3.2 Conservation Equations for the Liquid Phase

The mass conservation in liquid phase is equal the rate of volume because $p_l$ is constant and there is no flow inside the droplet.

$$\dot{m}^* = -\rho_l^* \frac{dV^*}{dt^*} \qquad (3.9)$$

In the gas phase, the enthalpy conservation is described by the following equation

$$\frac{\partial \rho_l^* \bar{h}^*}{\partial t^*} + \nabla \cdot \rho_l^* \mathbf{v}^* \bar{h}^* = \nabla \cdot k^* \nabla T^* + Q^* \omega^*$$

applying the assumptions for liquid phase in previous equation, we have

$$\frac{\partial \rho_l^* \bar{h}^*}{\partial t^*} = \nabla \cdot k^* \nabla T^* \qquad (3.10)$$

As the temperature is constant and uniform inside the droplet, then we can disregard the Eq. (3.10).

## 3.3 Dimensionless Equations

To describe conservation equations independently of the unit system, to eliminate some variables and do scale analysis, we need to rewrite these equations in dimensionless form. For this, some dependent and independent dimensionless variables are defined as follows

$$t_c \equiv \frac{t^*}{t_c^*} \qquad x \equiv \frac{r^*}{a_0^*} \qquad \rho \equiv \frac{\rho^*}{\rho_\infty^*} \qquad v \equiv \frac{v^*}{v_c^*} \qquad Y_O \equiv \frac{Y_{O*}}{Y_\infty^*} \qquad c_p \equiv \frac{c_p^*}{c_{p\infty}^*} = 1 \qquad L \equiv \frac{L^*}{c_p^* T_\infty^*}$$

$$T \equiv \frac{T^*}{T_\infty^*} \qquad k \equiv \frac{k^*}{k_\infty^*} \qquad \rho D \equiv \frac{\rho^* D^*}{\rho_\infty^* D_\infty^*} \qquad \nu \equiv \frac{\mu}{\rho} = \frac{\mu^*/\mu_\infty^*}{\rho^*/\rho_\infty^*}, \qquad Q \equiv \frac{Q^* Y_{F\infty}^*}{c_P^* T_\infty^* Le_F} \qquad h \equiv \frac{\bar{h}^*}{c_p^* T_\infty^*}$$

11

in which

$$t_c^* \equiv t_{vap}^* = \frac{(a_0^*)^2}{\alpha_\infty^* \epsilon} \qquad \epsilon \equiv \frac{\rho_\infty^*}{\rho_l^*} \qquad v_c^* \equiv \frac{\alpha_\infty^*}{a_0^*}$$

In this work, spherical symmetry is considered, so we must solve the problem using conservation equations in spherical coordinates. The divergence in spherical coordinate is

$$\nabla \cdot \mathbf{F}^* = \frac{1}{(r^*)^2} \frac{\partial}{\partial r^*} ((r^*)^2 F_r^*) + \frac{1}{r^* \sin\theta} \frac{\partial}{\partial \theta^*} (\sin\theta F_\theta^*) + \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi^*} (F_\phi)$$

and gradient is

$$\nabla f^* = \frac{\partial f^*}{\partial r^*} \hat{e}_r^* + \frac{1}{r^*} \frac{\partial f^*}{\partial \theta^*} \hat{e}_\theta^* + \frac{1}{r^* \sin\theta} \frac{\partial f^*}{\partial \phi^*} \hat{e}_\phi^*$$

The droplet combustion symmetry is independent of the variables $\theta$ and $\phi$. So

$$\nabla \cdot \mathbf{F}^* = \frac{1}{(r^*)^2} \frac{\partial}{\partial r^*} ((r^*)^2 F_r^*)$$

$$\nabla f^* = \frac{\partial f^*}{\partial r^*} \hat{e}_r^*$$

Applying the independent and dependent dimensionless variables in conservation equations of mass, specie i and energy, and rewriting in spherical coordinates, we have the dimensionless equations

$$\epsilon \frac{\partial}{\partial t} \rho + \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho v \right) = 0$$

$$\epsilon \frac{\partial \rho Y_i}{\partial t} + \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho Y_i v \right) = \frac{1}{Le_i} \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho D_i \frac{\partial Y_i}{\partial x} \right) + S_i Da \ \rho Y_F^{s_1} Y_O^{s_2} e^{-\Omega/T}$$

$$\epsilon \frac{\partial \rho T}{\partial t} + \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho v T \right) = \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 k \frac{\partial T}{\partial x} \right) + Le_F Q Da \rho Y_O^{s_2} Y_F^{s_1} e^{-\Omega/T}$$

$$\frac{da^2}{dt} = -2\beta$$

in which

$$S_O = \frac{s}{Y_O^*} \qquad S_F = 1 \qquad \dot{\omega} = Da \rho Y_F^{s_1} Y_O^{s_2} e^{-\Omega/T}$$

$$Da = \frac{B^*(a_c^*)^2}{\alpha_c^*} \frac{(Y_{Oc}^*)^{s_2} (Y_{Fc}^*)^{s_1}}{Y_{Fc}^*} \qquad \Omega = \frac{E^*}{R^* T_c^*} \qquad \beta = \frac{\lambda}{a}$$

Due to the fact that the Mach number is very small, the viscous dissipation is disregarded and the pressure gradient is zero. The energy conservation equation can be written in following form after replacing the dimensionless variables and

disregarding the chemical reaction

$$\epsilon \frac{\partial}{\partial t}(\rho h) + \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \rho v h\right) = \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 k \frac{\partial T}{\partial x}\right)$$

Here, $c_p = 1$ and $\epsilon << 1$, because the regime is low pressure, so the specific mass of the gas is less than that of the liquid. The transient term of the equations can be neglected. The mass conservation equation in dimensionless form, in simplify form, is

$$\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \rho v\right) = 0$$

Integrating the above equation, we have

$$x^2 \rho v = \lambda$$

in which $\lambda$ is the vaporization rate, which doesn't depend on space, only time

$$\lambda = \frac{\dot{m}^* c_p^*}{4\pi a_0^* k_c^*}$$

To complete the system of conservation equations, we have the gas equation of state in dimensional form

$$p^* = \rho^* R_g^* T^*$$

Dividing both side by $P_c^*$

$$\frac{p^*}{p_c^*} = \frac{\rho^* R_g^* T^*}{\rho_c^* R_c^* T_c^*}$$

P is constant through the space, so

$$\frac{p^*}{p_c^*} = 1$$

Therefore, the gas equation of state in dimensionless form is

$$1 = \rho T$$

In this mathematical formulation, transport properties are considered to be functions of temperature, according to

$$k = \rho \alpha = \rho D_i = \rho \nu = T^n$$

13

Finally, the system of conservation equations in dimensionless form for gas phase and liquid phase, respectively, is

$$x^2 \rho v = \lambda \tag{3.11}$$

$$\frac{\lambda}{x^2} \frac{\partial}{\partial x} Y_i = \frac{1}{Le_i} \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho \alpha \frac{\partial Y_i}{\partial x} \right) + S_i \dot{\omega} \tag{3.12}$$

$$\frac{\lambda}{x^2} \frac{\partial}{\partial x} T = \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho \alpha \frac{\partial T}{\partial x} \right) + Le_F Q \dot{\omega} \tag{3.13}$$

$$\rho T = 1 \tag{3.14}$$

$$\frac{da^2}{dt} = -2\beta \tag{3.15}$$

To determine ahead the energy conservation at the droplet surface, from which another boundary condition is specified, the enthalpy conservation equation is used,

$$\frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho v h \right) = \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho \alpha \frac{\partial T}{\partial x} \right) \tag{3.16}$$

## 3.4   Boundary Conditions

To solve conservation equations we need find boundary conditions. In this problem are three regions in domain that have many importance to describe the mathematics of droplet combustion. First, the droplet surface. There is no chemical reaction here and no oxidant is present. Second, the flame. Here all reagents are consumed and the temperature is $T_f$. Third, the infinite or ambient. In this region there is oxidant only and ambient temperature.

Now we go integrate the species conservation equation through the droplet surface, that is, from $a^-$ to $a^+$, in which $a^-$ is the liquid region and $a^+$ is the gas region. For $i = F$

$$\int_{a^-}^{a^+} \frac{\lambda}{x^2} \frac{\partial}{\partial x} Y_F dx = \int_{a^-}^{a^+} \frac{1}{Le_F} \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho D_F \frac{\partial Y_F}{\partial x} \right) dx$$

For $a^-$, $Y_F = 1$ and for $a^+$, $Y_{Fs} = e^{\gamma(1 - T_B/T_S)}$, in which $\gamma = L/R_g T_B$.

Therefore, the first boundary condition is

$$- \left[ \frac{x^2 \rho \alpha}{Le_F} \frac{\partial Y_F}{\partial x} \right]_{a^+} = \lambda (1 - Y_{Fs}) \tag{3.17}$$

Repeating the previous steps for Eq.(3.16)

$$\int_{a^-}^{a^+} \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 \rho v h \right) dx = \int_{a^-}^{a^+} \frac{1}{x^2} \frac{\partial}{\partial x} \left( x^2 k \frac{\partial T}{\partial x} \right) dx$$

Thus, we have the second boundary condition

$$x^2 k \frac{\partial T}{\partial x}\bigg|_{a^+} = \lambda L + x^2 k_l \frac{\partial T}{\partial x}\bigg|_{a^-} \tag{3.18}$$

in which L is the latent heat of vaporization, defined as

$$h(a^+) - h(a^-) = L$$

and

$$x^2 k_l \frac{\partial T}{\partial x}\bigg|_{a^-}$$

is the heat to inside the droplet. Due the fact the droplet temperature is $T_b$, there is no flux of heat to inside the droplet, therefore the term is equal to zero.

Finally, the boundary conditions are:

- Surface of drop, x = a

The mass flux that leaves the droplet is equal to the mass flux that evaporates

$$x^2 \rho \alpha \frac{\partial Y_F}{\partial x}\bigg|_{a^+} = Le_F \lambda (Y_{Fs} - 1) \tag{3.19}$$

and the heat transfer from the ambient atmosphere is employing for the vaporization and heating the droplet.

$$x^2 k \frac{\partial T}{\partial x}\bigg|_{a^+} = x^2 \rho \alpha \frac{\partial T}{\partial x}\bigg|_{a^+} = \lambda L \tag{3.20}$$

- Flame: $x = x_f$

Temperature equals temperature in flame condition, $T = T_f$, and all fuel and oxidizer are consumed, $Y_F = Y_O = 0$.

- Ambient atmosphere: x → ∞

Here, $Y_O = 1$, $Y_F = 0$ and $T = 1$

# 4 SHVAB - ZEL'DOVICH FORMULATION

The system of equations (3.12) and (3.13) is coupled through the transport coefficients and nonlinear by the reaction term, then its solution is found only numerically. Recognizing that $Y_F$, $Y_O$ and enthalpy are connected through stoichiometry, the equations for these dependent variables can be combined properly to remove the chemical term (DONINI, 2017). The resulting system of equations is known as the Schvab - Zel'dovich formulation. The chosen combinations lead to the equation for the mixture fraction Z and enthalpy excess H.

Here we assume that combustion occurs at the Burke-Schumann limit, $Y_F Y_0 = 0$. From the Schvab - Zel'dovich formulation in the Burke-Schumann limit, the equations for $Z$ and $H$ are able to describe the fuel side of the flame with the variables $(Y_F, T)$ and the oxidizer side with the variables $(Y_O, T)$ (FACHINI, 2006).

## 4.1 Without soot formation

The classical droplet combustion problem is described by,

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Y_O \\ Y_F \end{Bmatrix} - \begin{Bmatrix} 1 \\ 1/Le_O \\ 1/Le_F \end{Bmatrix}\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Y_O \\ Y_F \end{Bmatrix}\right) = \begin{Bmatrix} QLe_F \\ -S_O \\ -1 \end{Bmatrix}\dot{\omega} \qquad (4.1)$$

We will perform some algebric manipulations on these equations. First of all, we multiply the second line by $L_O$ and the third by $L_F$, leading to

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Le_OY_O \\ Le_FY_F \end{Bmatrix} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Y_O \\ Y_F \end{Bmatrix}\right) = \begin{Bmatrix} QLe_F \\ -S_OLe_O \\ -Le_F \end{Bmatrix}\dot{\omega}$$

Defining $S = S_OLe_O/Le_F$ and $\hat{\dot{\omega}} = Le_F\dot{\omega}$, the system of equations becomes

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Le_OY_O \\ Le_FY_F \end{Bmatrix} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\begin{Bmatrix} T \\ Y_O \\ Y_F \end{Bmatrix}\right) = \begin{Bmatrix} Q \\ -S \\ -1 \end{Bmatrix}\hat{\dot{\omega}}$$

The next algebric manipulations are the multiplication of the third line by $S$ and the subtraction of the resulting equation with the second line, using the definition of the mixture fraction $Z \equiv SY_F - Y_O + 1$, we have

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}(SLe_F Y_F - Le_O Y_O) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial}{\partial x}(SY_F - Y_O + 1)) = 0$$

Due the fact 1 is a constant, we can sum in partial derivative and rewriting in function of Z.

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}(SLe_F Y_F - Le_O Y_O) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial Z}{\partial x}) = 0$$

In the fuel side of the flame, the properties are $Y_O = 0$ and $Z = SY_F + 1$, then the equation for $Z$ is simplified to

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}(SLe_F Y_F) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial Z}{\partial x}) = 0$$

$$Le_F \frac{\lambda}{x^2}\frac{\partial}{\partial x}(Z) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial Z}{\partial x}) = 0$$

In oxidant side of the flame, the properties are $Y_F = 0$, $Z = -Y_O + 1$, then the equation for $Z$ is simplified to

$$Le_O \frac{\lambda}{x^2}\frac{\partial}{\partial x}(-Y_O) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial Z}{\partial x}) = 0$$

$$Le_O \frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \rho \alpha \frac{\partial Z}{\partial x}) = 0$$

In a generic form, the conservation equation for $Z$ can be written as

$$Le \frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \rho \alpha \frac{\partial Z}{\partial x}\right) = 0$$

with

$$Le(Z) = \begin{cases} Le_F, & Z \geq 1 \\ Le_O, & Z \leq 1 \end{cases}$$

The above equation can be rewritten even in a more generic form as

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} Le \, dz - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \rho \alpha \frac{\partial Z}{\partial x}\right) = 0 \tag{4.2}$$

Now we combining the all three equations of system to determine an equation for another conserved function, the excess of enthalpy, named as $H$. Multiplying the

first line of (4.1) by $(S+1)/Q$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left\{\begin{matrix}T(S+1)/Q\\Le_OY_O\\Le_FY_F\end{matrix}\right\} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\left\{\begin{matrix}T(S+1)/Q\\Y_O\\Y_F\end{matrix}\right\}\right) = \left\{\begin{matrix}(S+1)\\-S\\-1\end{matrix}\right\}\hat{\omega}$$

And adding the first line with second and third

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left(\frac{(S+1)T}{Q} + Le_OY_O + Le_FY_F\right) - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\left(\frac{(S+1)T}{Q} + Y_O + Y_F\right)\right) = 0$$

Defining $H = (S+1)T/Q + Y_F + Y_O)$ and applying in the first derivative, we have

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left\{H + Y_O(Le_O - 1) + Y_F(Le_F - 1)\right\} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = 0$$

In the fuel side of the flame, $Y_O = 0$ and $Y_F = (Z+1)/S$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[Z(Le_F - 1)/S\right] - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = 0$$

In the oxidant side of the flame, $Y_F = 0$ and $Y_O = 1 - Z$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} + \frac{\lambda}{x^2}\frac{\partial}{\partial x}Z(1 - Le_O) - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = 0$$

The generic form is

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z}Ndz = 0 \tag{4.3}$$

In which

$$N(Z) = \left\{\begin{matrix}(Le_F - 1)/S, & Z \geq 1\\1 - Le_O, & Z \leq 1\end{matrix}\right.$$

## 4.2 With soot formation

Here we include the chemical kinetics term for the soot formation in system (4.1)

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left\{\begin{matrix}T\\Y_O\\Y_F\end{matrix}\right\} - \left\{\begin{matrix}1\\1/Le_O\\1/Le_F\end{matrix}\right\}\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial}{\partial x}\left\{\begin{matrix}T\\Y_O\\Y_F\end{matrix}\right\}\right) = \left\{\begin{matrix}QLe_F\\-S_O\\-1\end{matrix}\right\}\dot{\omega} + \left\{\begin{matrix}-Q_{soot}Le_F\\0\\-1\end{matrix}\right\}\dot{\omega}_{soot} \tag{4.4}$$

Multiplying the second and third equations by $Le_O$ and $Le_F$ respectively, applying definitions for S and $\hat{\omega}$, multiplying third line by S and adding second line with third

19

line, we have

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left(SLe_FY_F - Le_OY_O\right) - \frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2\rho\alpha\frac{\partial}{\partial x}(SY_F - Y_O + 1)\right] = -S\hat{\omega}_{soot}$$

In the fuel region, $Y_O = 0$ and $SY_F = Z - 1$

$$Le_F\frac{\lambda}{x^2}\frac{\partial}{\partial x}(Z-1) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\rho\alpha\frac{\partial Z}{\partial x}) = -S\hat{\omega}_{soot}$$

$$Le_F\frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\rho\alpha\frac{\partial Z}{\partial x}) = -S\hat{\omega}_{soot}$$

In the oxidant region, $Y_F = 0$ and $-Y_O = Z - 1$

$$Le_O\frac{\lambda}{x^2}\frac{\partial}{\partial x}(Z-1) - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\rho\alpha\frac{\partial Z}{\partial x}) = -S\hat{\omega}_{soot}$$

$$Le_O\frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\rho\alpha\frac{\partial Z}{\partial x}) = -S\hat{\omega}_{soot}$$

In generic form

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} Le\,dz - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right) = -S\hat{\omega}_{soot} \qquad (4.5)$$

$$Le(Z) = \begin{cases} Le_F, & Z \geq 1 \\ Le_O, & Z \leq 1 \end{cases}$$

Multiplying second line by $Le_O$ and third line by $Le_F$, multiplying first line of system (4.4) by $(S+1)T/Q$, applying definitions for S and $\hat{\omega}$, and adding three equations of the system, we have

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[\frac{(S+1)}{Q}T + Le_OY_O + Le_FY_F\right] - \frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2\rho\alpha\frac{\partial}{\partial x}\left(\frac{(S+1)}{Q}T + Y_O + Y_F\right)\right] =$$

$$-\left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

Applying the definition of enthalpy excess, $H = (S+1)T/Q + Y_F + Y_O$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[H + Y_O(Le_O - 1) + Y_F(Le_F - 1)\right] - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = -\left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

In fuel side, $Y_O = 0$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[H + Y_F(Le_F - 1)\right] - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = -\left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

In which $Y_F = (Z-1)/S$

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\left[H + (Z-1)(Le_F - 1)/S\right] - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = -\left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = -\frac{(Le_F - 1)}{S}\frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

In the oxidant side, $Y_F = 0$ and $Y_O = Z - 1$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) = -(1 - Le_O)\frac{\lambda}{x^2}\frac{\partial Z}{\partial x} - \left[\frac{(S+1)Q_{soot}}{Q} + 1\right]\hat{\omega}_{soot}$$

In generic form

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} N dz = -\left[\frac{Q_{soot}}{Q}(S+1) + 1\right]\hat{\omega}_{soot} \quad (4.6)$$

$$N(Z) = \begin{cases} (Le_F - 1)/S, & Z \geq 1 \\ 1 - Le_O, & Z \leq 1 \end{cases}$$

The term of chemical kinetics related with the soot formation is

$$\hat{\omega}_{soot} = \lambda_{soot}\delta(x - x_{soot}) = \frac{\lambda_{soot}}{\lambda}\lambda\delta(x - x_{soot}) = \frac{\phi_m}{S}\lambda\delta(x - x_{soot}) \quad (4.7)$$

with

$$\phi_m = S\frac{\lambda_{soot}}{\lambda} \quad (4.8)$$

The value of $\phi_m$ is expressed in an empirical way, i.e., it is chosen artificially.

The amount of heat used in the soot generation is also modelled artificially, as

$$\left[\frac{Q_{soot}}{Q}(S+1) + 1\right]\hat{\omega}_{soot} = -\phi_q\lambda\delta(x - x_{soot})$$

in which

$$\phi_q \equiv \left[\frac{Q_{soot}}{Q}(S+1) + 1\right]\frac{\phi_m}{S}$$

Then, Eqs. (4.5) and (4.6)

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} Le\,dz - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right) = -\phi_m\lambda\delta(x - x_{soot}) \qquad (4.9)$$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} N\,dz = -\phi_q\lambda\delta(x - x_{soot}) \qquad (4.10)$$

## 4.3  Boundary conditions

Since the soot formation term is zero close to the droplet surface because $a = x < x_{soot}$, the integration of Eq. (4.9) from the liquid phase $(a^-)$ to the gas phase $(a^+)$ leads to

$$\lambda\int_{a^-}^{a^+}\frac{\partial}{\partial x}\left[\int_{Z_s}^{Z} Le\,dz\right]dx - \int_{a^-}^{a^+}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)dx = 0$$

Due the fact that we integrate in fuel side, we have

$$\int_{Z_s}^{Z} Le\,dz = Le_F(Z - Z_s)$$

and

$$Le_F\frac{\partial(Z - Z_S)}{\partial x} = Le_F\frac{\partial Z}{\partial x}$$

Therefore

$$Le_F\lambda\int_{a^-}^{a^+}\frac{\partial Z}{\partial x}dx - \int_{a^-}^{a^+}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)dx = 0$$

$$Le_F\lambda\left[Z\right]_{a^-}^{a^+} - \left[x^2\rho\alpha\frac{\partial Z}{\partial x}\right]_{a^-}^{a^+} = 0$$

$$Le_F\lambda[Z(a^+) - Z(a^-)] - \left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_{a^+} - \left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_{a^-} = 0$$

Since

$$Z(a^-) = S + 1 \qquad Z(a^+) = SY_{Fs} + 1 \qquad \left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_{a^-} = 0$$

then, the boundary condition for $Z$ at the droplet surface is

$$\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_{a^+} = Le_F S\lambda(Y_{Fs} - 1)$$

$$F_Z \equiv \left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_{a^+} \qquad (4.11)$$

To find the second boundary condition, we can combine the Eqs. (3.19) and (3.20). Rewriting these equations

$$\left(x^2 \rho \alpha \frac{\partial}{\partial x} \left\{ \begin{matrix} T \\ Y_F \end{matrix} \right\} \right)_{a^+} = \left\{ \begin{matrix} \lambda L \\ Le_F \lambda (Y_{Fs} - 1) \end{matrix} \right\}$$

Multiplying the first line by $(S+1)/Q$ and adding the second line, we have

$$\left(x^2 \rho \alpha \frac{\partial}{\partial x} \left( \frac{(S+1)T}{Q} + Y_F \right) \right)_{a^+} = \lambda L \frac{(S+1)}{Q} + Le_F \lambda (Y_{Fs} - 1)$$

In the fuel phase, $Y_O = 0$, that is, $H = (S+1)T/Q + Y_F$

$$\left(x^2 \rho \alpha \frac{\partial H}{\partial x}\right)_{a^+} = \lambda L \frac{(S+1)}{Q} + Le_F \lambda (Y_{Fs} - 1)$$

$$F_H \equiv \left(x^2 \rho \alpha \frac{\partial H}{\partial x}\right)_{a^+} \tag{4.12}$$

In the development of the model, the flux of $H$ will appear explicitly then for acquiring a compact mathematical formulation, it is defined $F_H$.

Therefore, the boundary conditions of gas phase is

- at the surface of droplet: $x = a$

$$H = \frac{(S+1)T_s}{Q} + Y_{Fs} \quad Z = SY_{Fs} + 1$$

$$F_Z \equiv \left(x^2 \rho \alpha \frac{\partial Z}{\partial x}\right)_{a^+} \quad F_H \equiv \left(x^2 \rho \alpha \frac{\partial H}{\partial x}\right)_{a^+}$$

- at the flame position: $x = x_f, Y_F = Y_O = T - T_f = 0$

$$H = \frac{(S+1)T_f}{Q} \quad Z = 1$$

- in the ambient atmosphere: $x \to \infty$, $Y_F = Y_O - 1 = T - 1 = 0$

$$H = \frac{(S+1)}{Q} \quad Z = 0$$

23

## 4.4 First analytical integration

Here we give the first steps to solve the equations in gaseous phase. Analysing equations (4.9) and (4.10) we realized that is possible to perform a analytical integration. To generalize the problem, we will consider the integration in the interval between the surface of the droplet and the arbitrary position x of the domain. The Eq.(4.9) is

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z}Ledz - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right) = -\phi_m\lambda\delta(x - x_{soot})$$

Multiplying both sides by $x^2/\lambda$ and integrating in the proposed domain

$$\left[\int_{Z_s}^{Z}Ledz\right]_a^x - \frac{1}{\lambda}\left[\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)\right]_a^x = -\phi_m\int_a^x x^2\delta(x - x_{soot})dx$$

Since

$$\left[\int_{Z_s}^{Z}Ledz\right]_a^x = \int_{Z_s}^{Z}Ledz - \int_{Z_s}^{Z(a)=Z_s} = \int_{Z_s}^{Z}Ledz$$

and

$$\frac{1}{\lambda}\left[\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)\right]_a^x = \frac{1}{\lambda}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right)_x - F_Z$$

then

$$\frac{\partial Z}{\partial x} = \frac{\lambda}{x^2\rho\alpha}\left[\int_{Z_s}^{Z}Ledz + \frac{F_Z}{\lambda} + \phi_m\int_a^x x^2\delta(x - x_{soot})dx\right] \tag{4.13}$$

Performing the same steps for Eq. (4.10)

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z}Ndz = -\phi_q\lambda\delta(x - x_{soot})$$

we have

$$H - H_s - \frac{1}{\lambda}x^2\rho\alpha\frac{\partial H}{\partial x} + \frac{1}{\lambda}F_H + \int_{Z_s}^{Z}Ndz = -\phi_q\int_a^x x^2\delta(x - x_{soot})dx$$

Therefore

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2\rho\alpha}\left[H - H_s + \frac{1}{\lambda}F_H + \int_{Z_s}^{Z}Ndz + \phi_q\int_a^x x^2\delta(x - x_{soot})dx\right] \tag{4.14}$$

in which

$$\tilde{H}_s \equiv H_s - F_H$$

$$= \left[ \frac{(S+1)T_s}{Q} + Y_{Fs} \right] - \left[ \frac{(S+1)}{Q}L - Le_F(1 - Y_{Fs}) \right]$$

$$= \frac{(S+1)T_s}{Q}(T_s - L) + Y_{Fs} + [Le_F(1 - Y_{Fs})]$$

$$= \frac{(S+1)T_s}{Q}(T_s - L) + Y_{Fs}(1 - Le_F) + Le_F$$

(4.15)

### 4.4.1 Analytical Solution

In the previous section it was possible to calculate the integrals of functions Z and H analytically. The second integration, however, is only possible if we adopt numerical methods. In this case, we assumed that the transport properties were dependent on the nth power of the temperature. In the case whereupon n = 0, we see that the differential equations of Z and H are reduced to a simpler case, which allows the analytical solution.

Remembering that

$$k = \rho\alpha = \rho D_i = \rho\nu = T^n$$

we can rewrite Eqs.(4.13) and (4.14) in the following form

$$\frac{\partial Z}{\partial x} = \frac{\lambda}{x^2 T^n} \left[ \int_{Z_s}^{Z} Le dz + F_Z + \phi_m \int_a^x x^2 \delta(x - x_{soot})dx \right]$$

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2 T^n} \left[ H - (H_s - F_H) + \int_{Z_s}^{Z} N dz + \phi_q \int_a^x x^2 \delta(x - x_{soot})dx \right].$$

Now, applying the conditions that we assume in this section, that is $n = 0$, the two equations above can be simplified, resulting in the following system of differential equations

$$\frac{\partial Z}{\partial x} = \frac{\lambda}{x^2} \left[ \int_{Z_s}^{Z} Le dz + F_Z + \phi_m \int_a^x x^2 \delta(x - x_{soot})dx \right],$$

(4.16)

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2} \left[ H - (H_s - F_H) + \int_{Z_s}^{Z} N dz + \phi_q \int_a^x x^2 \delta(x - x_{soot})dx \right].$$

(4.17)

In the next subsection, we will demonstrate the solutions of Eqs.(4.16) and (4.17). the strategy that will be adopted consists of dividing the integration domain into three parts: $a \le x < x_{soot}$, $x_{soot} \le x < x_f$ and $x_f \le x < \infty$. In each of these parts,

a solution for differential equations (4.16) and (4.17) will be found. The next step is to apply the boundary conditions and establish the continuity at $x = x_{soot}$ and $x = x_f$ in order to find the integration constants. The integrating factor method was chosen to solve each differential equation. The details of each solution will not be presented as it is beyond the focus of the work.

### 4.4.2 Analytical solution of Z

Starting with Eq. (4.16) and in the domain $a \leq x < x_{soot}$, we find

$$\int_{Z_s}^{Z} Le\,dz = Le_F(Z - Z_s), \quad F_Z = Le_F S(Y_{Fs} - 1), \tag{4.18}$$

$$\phi_m \int_a^x x^2 \delta(x - x_{soot})dx = 0. \tag{4.19}$$

Substituting the above expressions in Eq. (4.16), we find

$$\frac{\partial Z}{\partial x} = \frac{Le_F \lambda}{x^2}\left(Z - \tilde{Z}_s\right), \tag{4.20}$$

in which

$$\tilde{Z}_s \equiv Le_F Z_s - F_Z = S + 1. \tag{4.21}$$

Equation (4.20) can be integrated,

$$Z_1 = \tilde{Z}_s + C_1 e^{-Le_F \lambda/x} \qquad a \leq x < x_{soot}. \tag{4.22}$$

In the domain $x_{soot} \leq x < x_f$, the soot formation must be included in the formulation because is different from zero,

$$\tilde{\phi}_m \equiv \phi_m \int_a^x x^2 \delta(x - x_{soot})dx = \phi_m x_{soot}^2 = \phi_m \left(\frac{x_{soot}}{x_f}\right)^2 x_f^2 = \phi_m X_{sf}^2 x_f^2. \tag{4.23}$$

Thus, Equation (4.16) results in

$$\frac{\partial Z}{\partial x} = \frac{Le_F \lambda}{x^2}\left(Z - \tilde{Z}_s + \frac{\tilde{\phi}_m}{Le_F}\right) = \frac{Le_F \lambda}{x^2}\left(Z - \tilde{Z}_s + \tilde{\phi}_{m,F}\right),$$

and can be integrated

$$Z_2 = \tilde{Z}_s - \tilde{\phi}_{m,F} + C_2 e^{-Le_F \lambda/x} \qquad x_{soot} \leq x < x_f. \tag{4.24}$$

in which

$$\tilde{\phi}_{m,F} \equiv \frac{\tilde{\phi}_m}{Le_F} \tag{4.25}$$

In the domain, $x_f \leq x < \infty$ we find

$$\int_{Z_s}^Z Le\,dz = \int_{Z_s}^1 Le_F dz + \int_1^Z Le_O dz = Le_F[1 - (SY_{Fs} + 1)] + Le_O(Z - 1),$$

that leads to

$$\int_{Z_s}^Z Le\,dz + F_Z = Le_O \left[ (Z - 1) - \frac{Le_F S}{Le_O} \right], \tag{4.26}$$

and soot formation is given by (4.23). Thus, Equation (4.16) results in

$$\frac{\partial Z}{\partial x} = \frac{\lambda Le_O}{x^2} \left( Z - \tilde{Z}_{s(F,O)} + \tilde{\phi}_{m,O} \right),$$

and can be integrated,

$$Z_3 = \tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O} + C_3 e^{-Le_O \lambda / x} \qquad x_f \leq x < \infty. \tag{4.27}$$

in which

$$\tilde{Z}_{s(F,O)} \equiv \frac{SLe_F}{Le_O} + 1, \tag{4.28}$$

$$\tilde{\phi}_{m,O} \equiv \frac{\tilde{\phi}_m}{Le_O}. \tag{4.29}$$

In each integration, integration constants appeared, which were named $C_1$, $C_2$ and $C_3$. To find the expression for each of them, we need to impose continuity at $x_{soot}$ and $x_f$.

Applying the boundary condition in the ambient $Z(x \to \infty) = 0$, then $C_3 = -(\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})$ then

$$Z = \left( \tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O} \right) \left( 1 - e^{-Le_O \lambda / x} \right). \qquad x_f \leq x < \infty \tag{4.30}$$

Since the function $Z$ is continuous at the flame, then from Eqs.(4.24) and (4.27)

$$\tilde{Z}_s - \tilde{\phi}_{m,F} + C_2 e^{-Le_F \lambda / x_f} = \left( \tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O} \right) \left( 1 - e^{-Le_O \lambda / x_f} \right),$$

therefore

$$C_2 = \left[ \tilde{\phi}_{m,F} - \tilde{Z}_s + (\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})(1 - e^{-Le_O \lambda / x_f}) \right] e^{Le_F \lambda / x_f}.$$

Now we can rewrite Eq. (4.24) in $x_{soot} \leq x < x_f$ as follow

$$Z = \tilde{Z}_s - \tilde{\phi}_{m,F} + \left\{ \left[ \tilde{\phi}_{m,F} - \tilde{Z}_s + (\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})(1 - e^{-Le_O\lambda/x_f}) \right] e^{Le_F\lambda/x_f} \right\} e^{-Le_F\lambda/x}.$$
(4.31)

Once the constant $C_2$ has been verified, the next step is determined the constant $C_1$ imposing the continuity of the function $Z$ at the soot formation zone. Then, from Eqs (4.22) and (4.24) at $x = x_{soot}$

$$\tilde{Z}_s + C_1 e^{-Le_F\lambda/x_{soot}} = \tilde{Z}_s - \tilde{\phi}_{m,F} + C_2 e^{-Le_F\lambda/x_{soot}}$$

Manipulating the above equation, we find

$$C_1 = C_2 - \tilde{\phi}_{m,F} e^{Le_F\lambda/x_{soot}}.$$

The constant $C_2$ was calculated in previously, therefore

$$C_1 = (\tilde{Z}_{s(F,O)} - \tilde{Z}_s + \tilde{\phi}_{m,F} - \tilde{\phi}_{m,O}) e^{Le_F\lambda/x_f} + (\tilde{\phi}_{m,O} - \tilde{Z}_{s(F,O)}) e^{(Le_F - Le_O)\lambda/x_f} - \tilde{\phi}_{m,F} e^{Le_F\lambda/x_{soot}}$$

Now we can write (4.22) in $a \leq x < x_{soot}$ as follow

$$Z = \tilde{Z}_s + \left\{ \left[ \tilde{\phi}_{m,F} - \tilde{Z}_s + (\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})(1 - e^{-Le_O\lambda/x_f}) \right] e^{Le_F\lambda/x_f} - \tilde{\phi}_{m,F} e^{Le_F\lambda/x_{soot}} \right\} e^{-Le_F\lambda/x}$$
(4.32)

### 4.4.3  Analytical solution of H

Now we starting with Eq.(4.17) and analyze in the domain $a \leq x < x_{soot}$. Mathematically

$$\int_{Z_s}^{Z} N dz = N_F(Z - Z_s),$$
(4.33)

$$\phi_q \int_a^x x^2 \delta(x - x_{soot}) dx = 0.$$
(4.34)

We know that

$$H_s = \frac{(S+1)}{Q} T_s + Y_{Fs}, \quad F_H \equiv \left[ \frac{(S+1)}{Q} L - Le_F(1 - Y_{Fs}) \right],$$
(4.35)

$$N(Z) = \begin{cases} (Le_F - 1)/S, & Z \geq 1 \\ 1 - Le_O, & Z \leq 1 \end{cases},$$
(4.36)

Replacing the above conditions and condition (4.15) in Eq.(4.17), we find

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2} \left[ H - \tilde{H}_s + N_F(Z - Z_s) \right].$$

Defining $\hat{H}_s = \tilde{H}_s - N_F Z_s$

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2} \left[ H - \hat{H}_s + N_F Z \right]$$

in which $Z$ is the solution (4.22)

$$Z = \tilde{Z}_s + C_1 e^{-Le_F \lambda / x}.$$

The result of integration of above equation is

$$H = \hat{H}_s - \frac{(Le_F - 1)}{S} \left[ \tilde{Z}_s - \frac{C_1 e^{-Le_F \lambda / x}}{Le_F - 1} \right] + D_1 e^{-\lambda / x} \qquad a \le x < x_{soot} \qquad (4.37)$$

In the part of domain determined by $x_{soot} \le x < x_f$ we have

$$\phi_q \int_a^x x^2 \delta(x - x_{soot}) dx = \phi_q x_{soot}^2 = \phi_q X_{sf}^2 x_f^2 = \tilde{\phi}_q. \qquad (4.38)$$

Rewriting Eq.(4.17) with above conditions, we get

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2} \left[ H - \hat{H}_s + N_F Z + \tilde{\phi}_q \right],$$

in which $\hat{H}_s = H_s - F_H + N_F Z_s$ and

$$Z = \tilde{Z}_s - \tilde{\phi}_{m,F} + C_2 e^{-Le_F \lambda / x},$$

and the result of integration by parts of above differential equation is

$$H = \hat{H}_s + N_F \left( -\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F \lambda / x}}{Le_F - 1} - \tilde{\phi}_{q,N_F} \right) + D_2 e^{-\lambda / x} \qquad x_{soot} \le x < x_f, \qquad (4.39)$$

in which

$$\tilde{\phi}_{q,N_F} = \frac{\tilde{\phi}_q}{N_F}. \qquad (4.40)$$

Performing the same steps for part of domain defined by $x_f \le x < \infty$, we find

$$\int_{Z_s}^{Z} N dz = \int_{Z_s}^{1} N_F dz + \int_{1}^{Z} N_O dz = N_F(1 - Z_s) + N_O(Z - 1) = [N_F(1 - Z_s) - N_O] + N_O Z,$$

29

Making the substitutions in Eq.(4.17), we find

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2}\left(H - \tilde{H}_\infty + N_O Z + \tilde{\phi}_q\right),$$

in which

$$\hat{H}_\infty = H_s - F_H + N_F Z_s - N_F + N_O$$

and $Z$ is the solution (4.27)

$$Z = \tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O} + C_3 e^{-Le_O \lambda/x},$$

defining

$$\tilde{\phi}_{q,N_O} \equiv \frac{\tilde{\phi}_q}{N_O} \tag{4.41}$$

and integrating the partial differential equation of H in the domain $x_f \leq x < \infty$, we have

$$H = \hat{H}_\infty + N_O\left[\tilde{\phi}_{m,O} - \tilde{\phi}_{q,O} - \tilde{Z}_{s(F,O)}\right] + (\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})e^{-Le_O \lambda/x} + D_3 e^{-\lambda/x} \tag{4.42}$$

The constants $D_1, D_2$ and $D_3$ are integration constants. Applying the boundary condition in the ambient $H_\infty \equiv H(x \to \infty) = (S+1)/Q + 1$, $\tilde{\phi}_{m,O}$ and $\tilde{\phi}_{q,O}$ in Eq. (4.42), then

$$D_3 = H_\infty - \hat{H}_\infty + \left(-Le_O \tilde{Z}_{s(F,O)} + \tilde{\phi}_q + \tilde{\phi}_m\right),$$

and Eq. (4.42) in $x_f \leq x < \infty$ is writing as follow

$$H = \hat{H}_\infty + N_O\left[\tilde{\phi}_{m,O} - \tilde{\phi}_{q,O} - \tilde{Z}_{s(F,O)}\right] + (\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})e^{-Le_O \lambda/x}$$

$$+ \left[H_\infty - \hat{H}_\infty + \left(-Le_O \tilde{Z}_{s(F,O)} + \tilde{\phi}_q + \tilde{\phi}_m\right)\right]e^{-\lambda/x} \tag{4.43}$$

Since the function H is continuous at the flame, then Eqs. (4.39) and (4.42)

$$\hat{H}_s + N_F\left(-\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F \lambda/x_f}}{Le_F - 1} - \tilde{\phi}_{q,N_F}\right) + D_2 e^{-\lambda/x_f} =$$

$$\hat{H}_\infty + N_O\left(-\tilde{Z}_{s(F,O)} + \tilde{\phi}_{m,O} + \frac{(\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})e^{-Le_O \lambda/x_f}}{(1 - Le_O)} - \tilde{\phi}_{q,N_O}\right) + D_3 e^{-\lambda/x_f}.$$

Manipulating the above equality and isolating $D_2$, we find

$$D_2 = (\hat{H}_\infty - \hat{H}_s)e^{\lambda/x_f} - N_F\left(-\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F \lambda/x_f}}{Le_F - 1} - \tilde{\phi}_{q,N_F}\right)e^{\lambda/x_f}$$

$$+ N_O \left( -\tilde{Z}_{s(F,O)} + \tilde{\phi}_{m,O} + \frac{(\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})e^{-Le_O\lambda/x_f}}{(1 - Le_O)} - \tilde{\phi}_{q,N_O} \right) e^{\lambda/x_f} + D_3,$$

and Eq.(4.39) in $x_{soot} \leq x < x_f$ is writing as follow

$$H = \hat{H}_s + N_F \left( -\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F\lambda/x}}{Le_F - 1} - \tilde{\phi}_{q,N_F} \right)$$

$$+ \left[ (\hat{H}_\infty - \hat{H}_s)e^{\lambda/x_f} - N_F \left( -\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F\lambda/x_f}}{Le_F - 1} - \tilde{\phi}_{q,N_F} \right) e^{\lambda/x_f} \right.$$

$$\left. + N_O \left( -\tilde{Z}_{s(F,O)} + \tilde{\phi}_{m,O} + \frac{(\tilde{Z}_{s(F,O)} - \tilde{\phi}_{m,O})e^{-Le_O\lambda/x_f}}{(1 - Le_O)} - \tilde{\phi}_{q,N_O} \right) e^{\lambda/x_f} + D_3 \right] e^{-\lambda/x}$$

$$(4.44)$$

Once the constant $D_2$ has been verified, the next step is determined the constant $D_1$ imposing the continuity of the function H at the soot formation zone. Then, from Eqs. (4.37) and (4.39) at $x = x_{soot}$,

$$\hat{H}_s - N_F \left[ \tilde{Z}_s - \frac{C_1 e^{-Le_F\lambda/x_{soot}}}{Le_F - 1} \right] + D_1 e^{-\lambda/x_{soot}} =$$

$$\hat{H}_s + N_F \left( -\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F\lambda/x_{soot}}}{Le_F - 1} - \tilde{\phi}_{q,N_F} \right) + D_2 e^{-\lambda/x_{soot}}$$

Therefore, the constant $D_1$ is

$$D_1 = N_F \left[ \tilde{Z}_s - \frac{(C_2 - \tilde{\phi}_{m,F}e^{Le_F\lambda/x_{soot}})e^{-Le_F\lambda/x_{soot}}}{Le_F - 1} \right] e^{\lambda/x_{soot}}$$

$$+ N_F \left( -\tilde{Z}_s + \tilde{\phi}_{m,F} + \frac{C_2 e^{-Le_F\lambda/x_{soot}}}{Le_F - 1} - \tilde{\phi}_{q,N_F} \right) e^{\lambda/x_{soot}} + D_2,$$

and Eq.(4.37) in $a \leq x < x_{soot}$ is writing as follow

$$H = \hat{H}_s - N_F \left( \tilde{Z}_s - \frac{C_1 e^{-Le_F\lambda/x}}{Le_F - 1} \right)$$

$$+ \left[ N_F \tilde{\phi}_{m,F} e^{\lambda/x_{soot}} \left( \frac{Le_F}{Le_F - 1} \right) - N_F \tilde{\phi}_{q,N_F} e^{\lambda/x_{soot}} + D_2 \right] e^{-\lambda/x}. \qquad (4.45)$$

As we see, $\lambda$ is the eigenvalue of Eqs. (4.16) and (4.17). We want to know what influences the values of $x_f$, $T_f$ and $Y_{Fs}$ have on droplet combustion. For the solutions that we find, all other values, like for example $\tilde{\phi}_m$ and $\tilde{\phi}_q$, are input data. We must remember that $T_s = T_b$ and Clausius-Clapeyron equation not be needed. Therefore,

we solve just four algebraic equations to find the solutions of thus case. To make this, we will use numerical methods, like Newton-Raphson method for a system of nonlinear equations in the next work. However, the equations to be calculated will be exposed here.

The solution of Z in the region $a \leq x < x_{soot}$ describes a relation of $Y_{Fs}$ and $\lambda$. Applying the general solution (4.32) and assuming $\beta = \lambda/a$ and $X_f = x_f/a$ at droplet surface, $x = a$, we have

$$S(Y_{Fs} - 1) - \frac{(Le_F S - \tilde{\phi}_m)(Le_F - Le_O)}{Le_O Le_F} e^{Le_F \beta(1/X_f - 1)}$$

$$+ \left[\frac{(Le_F S - \tilde{\phi}_m)}{Le_O} + 1\right] e^{\beta[(Le_F - Le_O)/X_f - Le_F]} = 0. \tag{4.46}$$

The solution in $x_f \leq x < \infty$, $Z(x_f) = 1$, returns a relation of $x_f$ and $\lambda$, that is

$$Z_f = 1 = \frac{Le_F}{Le_O} S + 1 - \frac{\tilde{\phi}_m}{Le_O} - \left(\frac{Le_F S - \tilde{\phi}_m}{Le_O} + 1\right) e^{-Le_O \lambda/x_f},$$

and applying the definition of $\beta$ and $X_f$, we have

$$-\frac{Le_F}{Le_O} S + \frac{\tilde{\phi}_m}{Le_O} + \left(\frac{Le_F S - \tilde{\phi}_m}{Le_O} + 1\right) e^{-Le_O \beta/X_f} = 0. \tag{4.47}$$

The solution of H in the region $a \leq x < x_{soot}$ describes a relation of $T_s$, $Y_{Fs}$ and $\lambda$. Defining

$$\mathcal{S} = \frac{(Le_F S - \tilde{\phi}_m)}{Le_O} \tag{4.48}$$

$$\mathcal{H} \equiv \frac{(\mathcal{S} + 1)}{Q}(1 + L - T_b - Le_F Q) \tag{4.49}$$

and applying the general solution (4.45) at droplet surface, we have

$$-\frac{(\mathcal{S} + 1)}{Q} L - Y_{Fs} + 1 - S\frac{(Le_F S - \tilde{\phi}_m)(Le_F - Le_O)}{Le_O Le_F} e^{Le_F \beta}$$

$$+ S\left(\frac{Le_F S - \tilde{\phi}_m}{Le_O} + 1\right) e^{\beta[(Le_F - Le_O)/X_f + Le_F]} + S\left(\frac{\tilde{\phi}_m}{Le_F}\right) e^{Le_F \beta(a/x_{soot} - 1)} + \left(\frac{\tilde{\phi}_m}{S} - \tilde{\phi}_q\right) e^{\beta(a/x_{soot} - 1)}$$

$$+ \left(\frac{\mathcal{S} + 1}{S}\right) \left[(Le_O - 1)\mathcal{S}e^{\beta(1/X_f - 1)} + (\mathcal{S} + 1)e^{\beta((1 - Le_O)/X_f - 1)}\right] + (\mathcal{H} + \tilde{\phi}_q + \tilde{\phi}_m)e^{-\beta} = 0. \tag{4.50}$$

The solution of H in he region $x_f \leq x < \infty$ describer a relation for $x_f$ and $T_f$.

Applying the general solution (4.43) at flame position, we have

$$\frac{(S+1)(T_b-L)}{Q} + Y_{Fs}(1-Le_F) + Le_F + N_F S Y_{Fs} - \tilde{\phi}_q + N_O$$

$$-N_O \left( \frac{Le_F}{Le_O}S + 1 - \frac{\tilde{\phi}_m}{Le_O} - \frac{(Le_F S - \tilde{\phi}_m)/Le_O + 1}{1 - Le_O} e^{-Le_O \beta / X_f} \right) + (\mathcal{H} + \tilde{\phi}_q + \tilde{\phi}_m)e^{-\beta/X_f}$$

$$-\frac{(S+1)}{Q}T_f = 0. \tag{4.51}$$

The set of equations composed of Eqs.(4.46), (4.47), (4.50), and (4.51) will be solved by Newton-Raphson method for a system of a nonlinear equations in the next work.

# 5 CONCLUSIONS

Even though the project is not finalized, it was possible to obtain important results from which the understanding of the phenomenon of the droplet combustion is achieved and fundamental concepts are well settled leading to the analytical solution of the droplet combustion problem. The analysis of the scales permits the understanding of the time and length that characterize the problem, and the prove that justifies the simplification of the conservation equations according to the conditions imposed. Soot formation is described using a simplified mathematical model. The symmetry of the problem is spherical, so it was necessary to adopt spherical coordinates to rewrite the equations, which have radial, polar and azimuth coordinates. Due to the symmetry of the polar and azimuth coordinates, these were disregarded, leaving only the radial coordinate, i.e. a one-dimensional problem. The study of conservation equations establishes the necessary mathematical basis to describe the combustion of an isolated droplet. The nondimensionalization proceedure allows the conservation equations to be simplified according to the physics of the problem. Due to the fact that the Mach number is much less than the unit, the viscous dissipation and pressure gradient are disregarded from the energy conservation equation. As the ratio of gas density to liquid density is much smaller than one, the time derivative can be disregarded, which reduced the problem of solving ordinary differential equations. The equations that describe the liquid phase, or the fuel, are simplified by adopting that the internal velocity of the liquid in the drop is zero and that the pressure is constant. The droplet temperature is the boiling temperature, which eliminated the need to take heating process into account. The Shvab-Zel'dovich formulation employed in this work enabled the combination of the three equations that describe the problem and the elimination of the chemical reaction term, which is strong non-linear and raises the difficulty of solving. With that, it was possible to reduce the number of differential equations and system variables. The system of differential equations allowed an analytical integration, which was performed in this work. For the cases of no dependence of the transport coefficient on the temperature,i.e., the transport coefficients are constant, the system of ordinary partial differential equations for Z and H is solved analytically. A system of nonlinear algebraic equations for the problem properties is found and will be solved numerically. At the end of this stage, the characteristic scales, a model of the combustion of an isolated droplet with soot formation are determined. The next step is to solve numerically with a home computer code the resulting system of nonlinear algebraic equations for the properties. The results of this analysis will be submitted to a journal of the combustion science area.

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