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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ABSTRACT

The present work 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 next step will be to implement a computational code to solve the numerical integration, in addition to implementing the heat transfer by radiation.

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

FORMULAÇÕES DE SHVAB-ZELDOVICH E FLAMELET APLICADAS À COMBUSTÃO QUASE ESTÁVEL DE GOTÍCULA, COM FORMAÇÃO DE FULIGEM E TRANSFERÊNCIA RADIATIVA DE CALOR

RESUMO

O presente trabalho estuda teoricamente a combustão quase estável de uma gotícula 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 estável é justificado pelo fato de que a inércia térmica da fase gasosa próxima à gotícula é muito menor que a da fase líquida, de modo que o ambiente se adapta muito mais rapidamente que a gotícula. A temperatura de ebulição foi considerada para toda a gotícula, 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-Zel'dovich, 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 gotícula 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. O próximo passo será implementar um código computacional para resolver a integração numérica, além de implementar a transferência de calor por radiação.

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
ρ	–	Density
α	–	Thermal diffusivity
τ	–	Contact force tensor
ω	–	Chemical reaction term
ν	–	Cinematic Viscosity
μ	–	Dynamic Viscosity
λ	–	Nondimensional vaporisation rate
$\dot{\omega}$	–	Dimensionless chemical reaction term
$\dot{\omega}_{soot}$	–	Nondimensional chemical reaction term for soot
ϕ_m	–	Mass of soot
ϕ_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 ρ_∞^*, thermal conductivity k_∞^*, constant pressure specific heat c_P^*. The gas temperature and the mass fraction of the oxidant are kept constant at T_∞^* and $Y_{O\infty}^*$.

In this work, the superscript "*" indicates the variable in dimensional form and the subscript ∞ 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.

$$C_xH_y + (x + y/4)O_2 \rightarrow xCO_2 + y/2H_2O \tag{2.1}$$
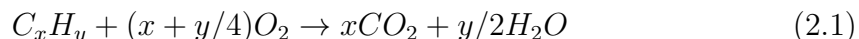
An ideal condition means that the oxygen content of the mixture is sufficient to react with all the fuel. In practice, the conditions are different from the ideal, that is, if the oxygen present is not sufficient to fully convert the fuel according to Eq. (2.1), and if the fuel pyrolysis to occur, the 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.

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

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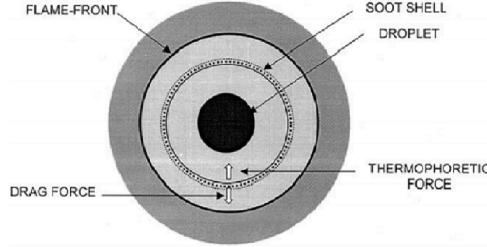
In this work, an infinitely fast reaction is considered, then the soot particles are formed only by the pyrolysis of fuel in the region of temperature around $1200K$, given by a first order reaction $F \rightarrow Soot$. The term of chemical kinetics related with the soot formation is modelled in simple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

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

in which λ_{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

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

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

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

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

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

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

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 Σ_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, Σ 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 ρ_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

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

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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

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

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

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

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

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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 θ and ϕ. 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 λ 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

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

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)

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

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Thus, we have the second boundary condition

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

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

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

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

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

- 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

Solving the equations (3.12) and (3.13) is difficult due to the presence of nonlinear terms. Recognizing that Y_F, Y_O and system enthalpy are connected through stoichiometry, these terms can be combined stoichiometrically, such that resulting term is not affected by chemical reactions (DONINI, 2017).Then these equations lead to two linear equations as a function of Z and H, where Z is the mixing fraction and H is the enthalpy excess.

Here we assume that combustion occurs at the Burke-Schumann limit. To describe the combustion problem, we use the Schvab - Zel'dovich formulation, which makes no distinction between the fuel and oxidant-containing region. Such formulation is obtained by combining the equations (3.12) and (3.13) (FACHINI, 2006)

4.1 Without soot formation

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

Multiplying the second line by L_O and the third by L_F

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

And defining $S = S_OLe_O/Le_F$ and $\hat{\dot\omega} = Le_F\dot\omega$, we have

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

Multiplying the third line by S, subtracting the second line and defining the mixture fraction function such $Z \equiv SY_F - Y_O + 1$, we have

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

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

function of Z.

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

In the fuel side of the flame, $Y_O = 0$ and $Z = SY_F + 1$.

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

Since $SY_F = Z - 1$. Therefore

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

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

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

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

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

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

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 $(S+1)/Q$

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

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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

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

4.2 With soot formation

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

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

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 line, we have

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

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

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

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

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

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 $Y_F = (Z - 1)/S$

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

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

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

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

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

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

The value of $\phi_m \equiv \lambda_{soot}/\lambda$ 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)

$$\frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} Le dz - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial Z}{\partial x}\right) = -\phi_m\lambda\delta(x - x_{soot}) \quad (4.7)$$

$$\frac{\lambda}{x^2}\frac{\partial H}{\partial x} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\rho\alpha\frac{\partial H}{\partial x}\right) + \frac{\lambda}{x^2}\frac{\partial}{\partial x}\int_{Z_s}^{Z} N dz = -\phi_q\lambda\delta(x - x_{soot}) \quad (4.8)$$

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. (4.7) 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

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

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

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

$$F_Z \equiv \left(x^2 \rho\alpha \frac{\partial Z}{\partial x}\right)_{a^+} \tag{4.9}$$

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, $H = (S+1)T/Q + Y_F$

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

$$F_H \equiv \left(x^2 \rho \alpha \frac{\partial H}{\partial x}\right)_{a^+} \tag{4.10}$$

Therefore, the boundary conditions of gas phase is

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

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

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

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

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

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

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

4.4 First analytical integration

Here we give the first steps to solve the equations in gaseous phase. Looking at the equations (4.7) and (4.8) 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.(4.7) is

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

Multiplying both sides by x^2/λ and integrating in the proposed domain

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

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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

$$\frac{\partial Z}{\partial x} = \frac{\lambda}{x^2\rho\alpha}\left[\int_{Z_s}^{Z} Ledz + \frac{F_Z}{\lambda} + \phi_m\int_a^x x^2\delta(x - x_{soot})dx\right] \qquad (4.11)$$

Performing the same steps for Eq. (4.8)

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

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

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2\rho\alpha}\left[H - H_s + \frac{1}{\lambda}F_H + \int_{Z_s}^{Z} Ndz + \phi_q\int_a^x x^2\delta(x - x_{soot})dx\right] \qquad (4.12)$$

For the case that $Le_F = Le_O = 1$ we can make some simplifications in the equations above. These simplifications are

$$\int_{Z_s}^{Z} Ledz = \int_{Z_s}^{1} Le_F dz + \int_1^{Z} Le_O dz = Le_F(1 - Z_s) + Le_O(Z - 1) = Z - Z_s$$

$$\frac{1}{\lambda}F_Z = S(Y_{Fs} - 1)$$

$$\int_{Z_s}^{Z} Ndz = \int_{Z_s}^{1}\frac{Le_F - 1}{S}dz + \int_1^{Z}(1 - Le_O)dz = \int_{Z_s}^{1}\frac{1 - 1}{S}dz + \int_1^{Z}(1 - 1)dz = 0$$

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

Rewriting the Eqs. (4.11) and (4.12)

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

$$\frac{\partial H}{\partial x} = \frac{\lambda}{x^2\rho\alpha}\left[H - H_s + L\frac{(S + 1)}{Q} + (Y_{Fs} - 1) + \phi_q\int_a^x x^2\delta(x - x_{soot})dx\right]$$

5 CONCLUSIONS

Even though the project is not finalized, it was possible to obtain important results from which the understanding of the phenomena of droplet combustion is achieved and fundamental concepts are well settled leading to a rigorous solution of the droplet combustion problem. The analysis of the scales permits the understanding of the time and length that characterize the problem, in addition to justifying 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, that is, a one-dimensional problem. The study of conservation equations established the necessary mathematical basis to describe the combustion of an isolated droplet. The nondimensionalization proceedure allowed 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 have been disregarded from the energy conservation equation. As the ratio of gas density to liquid density, ϵ, is much smaller than one, time derivatives could be disregarded, which reduced the problem of solving ordinary differential equations. The equations that describe the liquid phase, or the fuel, have been simplified by adopting that the internal speed 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 time 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. Furthermore, the Shvab-Zeldovich formulation does not distinguish between the fuel-containing region and the oxidant-containing region. The system of differential equations allowed an analytical integration, which was performed in this work. For this, it was necessary to find the boundary conditions on the surface of the droplet. At the end of the first stage, it was possible to determine the characteristic scales, deduce the conservation equations, model the combustion of an isolated droplet with soot formation and consolidate the theoretical basis. The next step is to solve numerically, using home computer code, the resulting differential equations, to implement radiative heat transfer and to obtain data that will allow the publication of the work in a period of relevance in the area.

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