

NUMERICAL COMBUSTION MODELING OF A LINEAR ARRAY OF GASEOUS FUEL POCKETS WITH NONUNITARY LEWIS NUMBER

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Abstract. This work presents the numerical combustion modeling of an infinite linear array of gaseous fuel pockets in a stagnant oxidizing environment under microgravity conditions. The gas pocket combustion is described using the generalized Shvab-Zel'dovich formulation with nonunitary Lewis number. The combustion process is considered isobaric and the fluid motion is induced by density gradients due to the heat and mass transfer processes. The model is based on mass, momentum, excess enthalpy and mixture fraction conservation equations and considers the Burke-Schumann reaction mechanism and ideal gas behavior. The thermophysical properties, except the density, are assumed constant. The Finite Volume Method is employed in the numerical solution, using a generalized system of coordinates. A non-staggered grid is used and the SIMPLEC algorithm is employed to solve the modified pressure-velocity coupling. The Lewis number effects on flame behavior and on the fuel consumption are analysed.

Keywords: combustion, gas pocket, diffusion flame, Lewis number

1. INTRODUCTION

Some basic and applied research have been devoted to gas fuel pocket (or cloud) combustion problems (Sánchez-Tarifa *et al.*, 1972, Johari and Motevalli, 1993, Librovich *et al.*, 1999, Daou, 1998, Daou and Rogg, 1998, Caldeira *et al.*, 2004, 2008). These works were concerned with fundamental non-premixed combustion phenomena modeling as well as flame dynamics. Furthermore, in engineering systems as diesel engines, gas turbines and rocket engines, liquid fuel droplets are injected in supercritical environments and rapidly reach supercritical conditions (Zhu and Aggarwal, 2000). Under such conditions, the droplets behave like dense gas pockets (Sánchez-Tarifa *et al.*, 1972, Daou, 1998, Daou and Rogg, 1998, Caldeira *et al.*, 2004, 2008).

Due to complexity of the spray combustion phenomena, single droplet and droplet arrays have been studied (Annamalai and Ryan, 1992, Gliver and Abraham, 1996, Bellan, 2000). The effects of droplet interactions are known to play an important role in the vaporization and combustion of droplet arrays (Imaoka and Sirignano, 2005). The linear droplet (or gas pocket) array is a simple arrangement that retains information about the interactions effects on the flame dynamics (Leiroz and Rangel, 1997, Caldeira *et al.*, 2004, 2008).

In diffusive flame combustion modeling, the Burke-Schumann reaction mechanism has been used to avoid the detailed chemistry, preserving important aspects of the flame dynamics (Matalon, 2009). The traditional Shvab-Zel'dovich model considers the Burke-Schumann reaction mechanism with unitary Lewis number (Daou and Rogg, 1998, Caldeira *et al.*, 2008). Mathematically, these assumptions simplify the combustion model, reducing the number of differential conservation equations. However, the unitary Lewis number assumption is not realistic in many practical situations. To overcome this limitation, extensions of the Shvab-Zel'dovich formulation have been proposed including the nonunitary Lewis number (Liñán and Williams, 1993, Fachini *et al.*, 1999, Sirignano, 2007, Fachini, 2008).

The numerical combustion modeling of an infinite linear array of gaseous fuel pockets with nonunitary Lewis number is shown in this work. The Finite Volume Method is employed in the numerical solution. A non-staggered grid is used and the modified pressure-velocity coupling is solved by the SIMPLEC algorithm. The effects of the Lewis number on the flame behavior and on the fuel consumption are analyzed. To verify the quality of the model and the numerical solution, results for unitary Lewis number are compared with benchmark results available in the literature.

2. PHYSICAL AND MATHEMATICAL MODEL

The physical model considered here involves the combustion of an infinite linear array of gaseous fuel pockets. The combustion process is considered isobaric and the thermophysical properties, except the density, are assumed constant. The density is temperature dependent through the application of the ideal gas equation of state. The model considers the Burke-Schumann reaction mechanism and ideal gas behavior. The combustion is represented by a single irreversible one-step reaction of the form presented in Eq. (1), where s is the stoichiometric coefficient.



The fluid motion is induced by density gradients due to the heat and mass transfer processes (Daou, 1998, Daou and Rogg, 1998, Caldeira, 2004, Caldeira *et al.*, 2008). The model is based on mass, momentum, excess enthalpy and mixture fraction conservation equations (Liñán and Williams, 1993, Fachini *et al.*, 1999).

In the initial condition, the gaseous fuel pocket array, with mono-sized, spherical and equidistant pockets, is assumed to be inside an oxidant environment. The temperature inside the gaseous pockets and the environment temperature are supposed constant. However, the initial values of the pocket and the environment temperatures could be different. Moreover, the velocity field is null in role domain.

The dimensionless form of the conservation equations of the mass, momentum, energy, and mass fraction of the reactants are presented, respectively, in Eqs.(2-6). In the momentum equations, Re is the Reynolds number and p is the modified pressure defined by the addition of the thermodynamic pressure and the volumetric expansion terms (Daou, 1998, Daou and Rogg, 1998, Caldeira *et al.*, 2004, 2008). In the energy and in the mass fraction conservation equations, Pe is the Peclet number, q is the dimensionless heat of reaction, Ω is the dimensionless fuel consumption rate, Le_o is the oxidant Lewis number and Le_f is the fuel Lewis number. The dependent variables of the equations system are: density (ρ), velocity vector (\mathbf{u}), temperature (T), fuel mass fraction (Y_f) and oxidant mass fraction (Y_o).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \frac{1}{Re} \nabla \cdot (\nabla \mathbf{u}) - \nabla p \quad (3)$$

$$\frac{\partial}{\partial t} (\rho T) + \nabla \cdot (\rho \mathbf{u} T) = \frac{1}{Pe} \nabla^2 T + q \Omega \quad (4)$$

$$\frac{\partial}{\partial t} (\rho Y_f) + \nabla \cdot (\rho \mathbf{u} Y_f) = \frac{1}{Le_f Pe} \nabla^2 Y_f - \Omega \quad (5)$$

$$\frac{\partial}{\partial t} (\rho Y_o) + \nabla \cdot (\rho \mathbf{u} Y_o) = \frac{1}{Le_o Pe} \nabla^2 Y_o - s \Omega \quad (6)$$

The present work considers that the superscript “+” refers to dimensional variables or parameters, the subscript “f” is related to the fuel, the subscript “o” is related to the oxidant and the symbol “ ∞ ” is associated to quantities evaluated in a region far from the gas pocket array. The dimensionless procedure is based in the initial gas pocket radius, R_0^+ , in the characteristic velocity, $u_c^+ = \mu_\infty^+ / \rho_\infty^+ R_0^+$, and in the thermophysical properties evaluated far from the array. The dimensionless independent variables are the spherical coordinates, $R = R^+ / R_0^+$ and θ (or the cylindrical coordinates $r = r^+ / R_0^+$ and $z = z^+ / R_0^+$) and the time, $t = u_c^+ t^+ / R_0^+$. The dimensionless dependent variables are defined as: the velocity vector, $\mathbf{u} = \mathbf{u}^+ / u_c^+$, the density, $\rho = \rho^+ / \rho_\infty^+$, the temperature, $T = T^+ / T_\infty^+$, and the modified pressure, $p = p^+ / (\rho_\infty^+ u_c^+ u_c^+)$. The dimensionless numbers are $Re = \rho_\infty^+ u_c^+ R_0^+ / \mu_\infty^+$, $Pe = \rho_\infty^+ c_{p,\infty}^+ u_c^+ R_0^+ / k_\infty^+$, $Le_f = k_\infty^+ / (\rho_\infty^+ c_{p,\infty}^+ D_f^+)$ and $Le_o = k_\infty^+ / (\rho_\infty^+ c_{p,\infty}^+ D_o^+)$, where μ is the dynamic viscosity, k is the thermal conductivity, c_p is the specific heat at constant pressure and D is the mass diffusivity. The dimensionless fuel consumption and heat release are, respectively, $\Omega = R_0^+ \Omega^+ / (\rho_\infty^+ u_c^+)$ and $q = q^+ / (c_{p,\infty}^+ \cdot T_\infty^+)$. Then, applying the dimensionless procedure $Re = 1$.

The density is temperature dependent through the application of the ideal gas equation of state as shown in Eq.(7). This dimensionless equation is obtained considering the isobaric combustion process.

$$\rho = T^{-1} \quad (7)$$

The system of equations Eq.(2-6) is simplified by the generalized Shvab-Zel'dovich assumptions. The generalized Shvab-Zel'dovich variables (Liñán and Williams, 1993), excess enthalpy (H) and mixture fraction (F) are defined, respectively, in Eq.(8) and in Eq.(9).

$$H = \frac{(s+1)}{q} T + Y_o + Y_f \quad (8)$$

$$F = s \cdot Y_f - Y_o + 1 \quad (9)$$

The Burke-Schumann reaction mechanism establishes a thin diffusive flame. The flame is, mathematically, represented by a surface with mixture fraction equal to one. The flame divides the domain in two regions: one region with fuel, products and inert chemical species, and the other region with oxidant, products and inert chemical species. In

some cases, the inert chemical species are not present. The flame is a surface that acts as a source of energy and products and a sink of reactants.

The definitions of the generalized Shvab-Zel'dovich variables describe the algebraic operations required to simplify the conservation equations of energy and mass fractions, eliminating the source terms. Such procedure leads to the conservation equation of the excess enthalpy and mixture fraction shown in Eq.(10-13).

$$\frac{\partial}{\partial t}(\rho F) + \nabla \cdot (\rho \mathbf{u} F) = \frac{1}{L Pe} \nabla^2 F \quad (10)$$

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \mathbf{u} H) = \frac{1}{Pe} \nabla^2 H - \frac{N}{L Pe} \nabla^2 F \quad (11)$$

$$L = \begin{cases} Le_f, & F > 1 \\ Le_o, & F < 1 \end{cases} \quad (12)$$

$$N = \begin{cases} \frac{Le_f - 1}{s}, & F > 1 \\ 1 - Le_o, & F < 1 \end{cases} \quad (13)$$

In the generalized Shvab-Zel'dovich formulation, the dependent variables of the conservation equation system are reduced to density, velocities, excess enthalpy and mixture fraction. The temperature and the reactants mass fractions are evaluated using the Eq.(8-9).

The infinite linear array of gaseous fuel pockets is a special arrangement with a simple mathematical domain. The symmetries of the problem under microgravity conditions turn this configuration attractive in the theoretical study of interactive gas pockets (or droplets) combustion (Leiroz and Rangel, 1997, Caldeira, 2004, Caldeira *et al.*, 2008). These symmetries are shown in Fig 1. In this figure, b^+ is the half-interpocket distance and c^+ is the cylindrical radial truncation position of the domain where the infinity boundary conditions are applied. The spherical coordinated system (R^+, θ^+) and the cylindrical coordinate system (r^+, z^+) , both with origin positioned in the center of the gas pocket, are represented in Fig. 1.

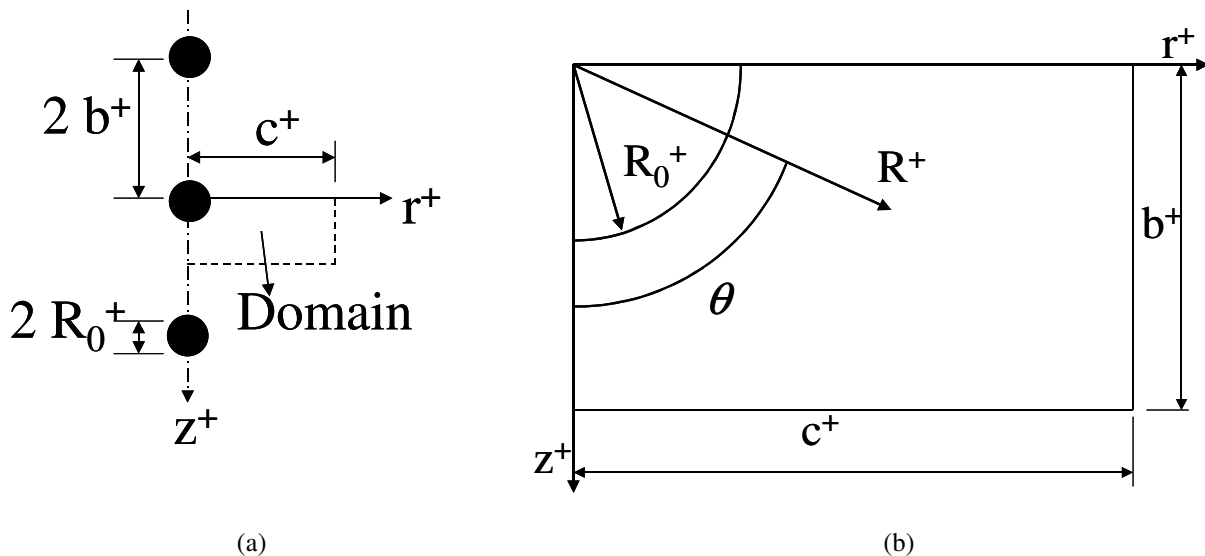


Figure 1. Physical model: (a) geometry and (b) simplified domain (Caldeira *et al.*, 2004).

Homogeneous flux boundary conditions are applied for the dependant variables along the boundaries as a result of the symmetries and the infinity condition of the problem. In the initial conditions, the excess of enthalpy and the mixture fraction variables are obtained specifying the initial temperature and reactants mass fractions.

It is important to note that the proposed model can be applied to some engineering problems where the oxidant constitutes the gaseous pockets and the fuel constitutes the environment.

3. NUMERICAL SOLUTION

The conservation equations are transformed to a generalized coordinated system (Thompson *et al.*, 1985, Maliska, 1995). The finite volume method is employed in a non-staggered grid (Maliska, 1995) and the (modified) pressure-velocity coupling is solved by the SIMPLEC algorithm (Van Dormaal and Raithby, 1984). The WUDS (Raithby and

Torrance, 1974) is used as the interpolation function in an implicit scheme. The linear systems of equations are solved by the GMRES algorithm (Press *et al.*, 1992).

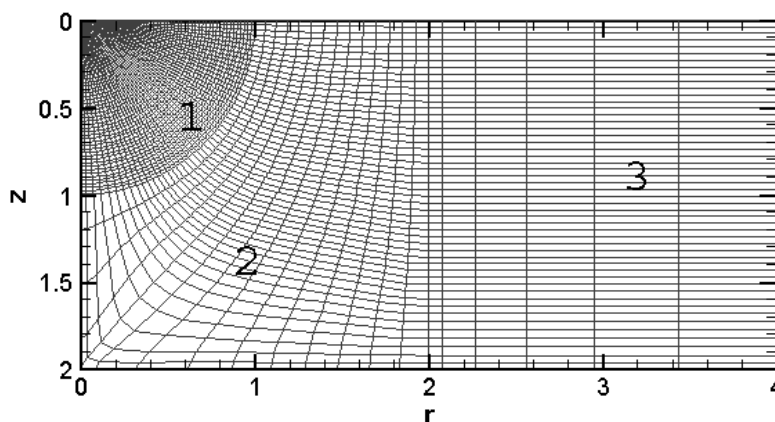


Figure 2. Typical hybrid-mesh (Caldeira *et al.*, 2004).

Figure 2 presents a typical mesh employed in this work. The domain and the mesh are divided in three regions. In the regions 1 and 3 the mesh is generated algebraically and in region 2 the mesh is generated numerically (Caldeira *et al.*, 2004). This mesh is based on: the spherical characteristics of the initial gas pocket condition, describing them in region 1; the cylindrical characteristics of the linear array, which is found in region 3; and the streamlines of an infinity array of source points in the region 2. Nevertheless, the region 1 can be greater than the initial gas fuel pocket (Caldeira *et al.*, 2004).

Two strategies can be adopted to simulate the isolated gas pocket condition: in the first one large values of the parameter b are used and in the second one an algebraically generated mesh with only a large region 1 represented in Fig. 2 is used. However, to guarantee no interaction effects on the combustion process and to reduce the computational cost, the second strategy is adopted for isolated gas pocket simulations.

Numerical convergence problems could appear at the end of the combustion process. Strong velocity gradients are induced in the vicinity of the flame by the thermal expansion of the gas. At the end of the combustion process, the flame goes toward the pocket center that is a stagnation point. Nevertheless, the proposed flame model fails at the end of the combustion process, because the model does not consider the extinction of the reaction (Caldeira *et al.*, 2004, 2008). To overcome these problems the numerical solution was stopped before the fuel is totally consumed.

4. RESULTS

In present work, the mass of fuel is evaluated using

$$m_f(t) = \int_{V_{st}} \left(\frac{F-1}{s} \right) \rho dV \quad (14)$$

where V is the volume and V_{st} is the volume limited by the flame.

The limiting case of gas pocket array combustion with infinity half-interpocket distance, $b \rightarrow \infty$, (or the isolated gas pocket combustion) is used to compare the solutions obtained with the proposed Generalized Shvab-Zel'dovich (GSZ) model with reference solutions (Daou and Rogg, 1998, Caldeira *et al.*, 2004). These solutions are reported in Fig. 3 and 4. The algebraic mesh with 160×20 volumes is employed in isolated gas pocket simulation. The physical conditions for isolated gas fuel pocket combustion consider: $Le_f = 1$, $Le_o = 1$, $Pe = 1$, $s = 0.25$, $q = 2$ and the initial fuel temperature equal to 10% of the initial oxidant temperature. The values of these parameters were chosen considering the reference work (Daou and Rogg, 1998). Furthermore, no inert chemical species are considered.

Figure 3 shows the evolution along the time of the normalized mass of fuel for isolated gas pocket combustion cases. The maximum absolute discrepancy between the results shown in Figures 3 are smaller than 0.01. The fuel consumption can be analyzed, qualitatively, observing the inclination of the curves of the normalized mass of fuel. As expected, the fuel consumption is more intense in earlier times of the combustion process, because of the greater concentration of reactants in the initial condition. Nevertheless, the proposed model is not able to represent the ignition and extinction phenomena.

The flame position r_{st} and z_{st} , respectively, on the cylindrical coordinates axis r and z and the average radius of the flame R_{st} are compared in Figure 4. These results reveal that the r_{st} and z_{st} curves are coincident, indicating the spherical shape of the flame. This shape is physically explained by the spherical symmetry of the problem. Moreover, the

maximum relative discrepancy between the curves in the Figure 4 is smaller than 2.5%. In this figure, the flame moves in the environment direction, reaching a maximum stand-off. This flame movement is induced by the high fuel concentration established in the initial condition. But, along of the time the fuel is consumed and the flame recedes towards the pocket center. The differences between the results obtained with the proposed model and the ones presented by Daou and Rogg (1998) can be attributed to the forced convection, which was not considered in the present work. “The work of Daou and Rogg (1998) is devoted to the combustion of one supercritical fuel droplet moving in an oxidizing atmosphere. So, the results of Daou and Rogg (1998) for low Reynolds number ($Re = 0.1$) are compared here with the results reached with the present model that consider the stagnant system as the initial condition” (Caldeira *et al.*, 2004). However, the Reynolds number has different definitions in present work and in Daou and Rogg (1998).

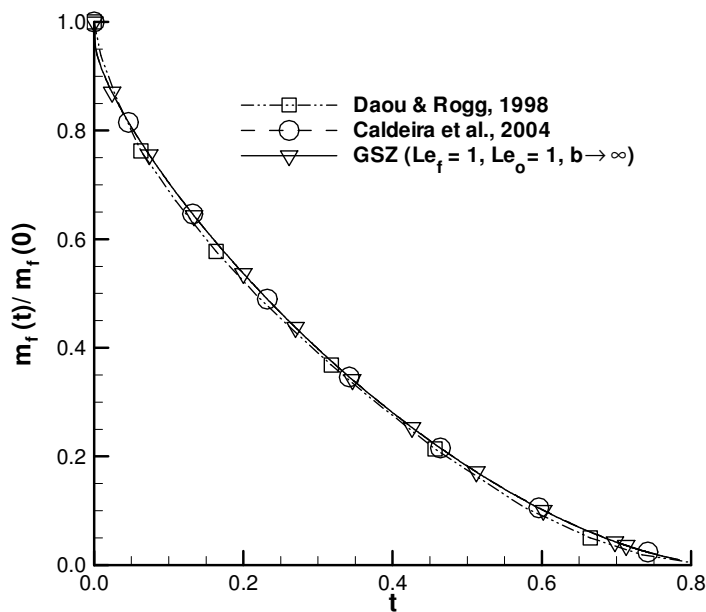


Figure 3. Normalized mass of fuel ($Le_f = 1, Le_o = 1, b \rightarrow \infty$).

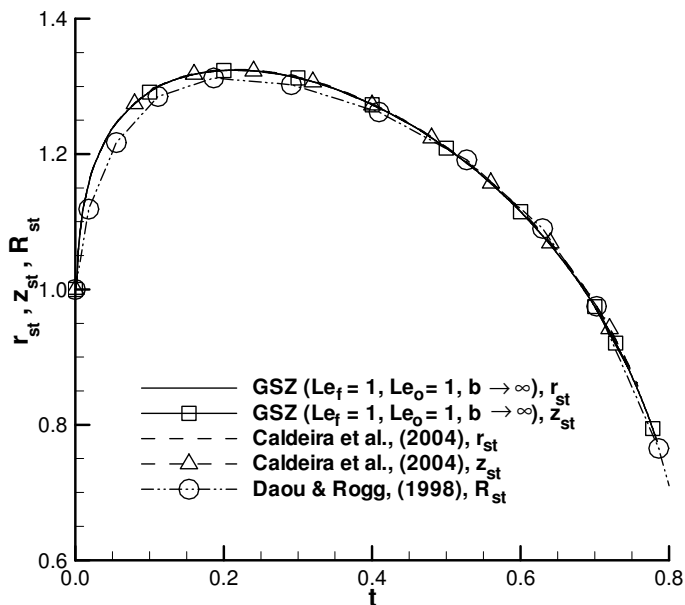


Figure 4. Flame behavior ($Le_f = 1, Le_o = 1, b \rightarrow \infty$).

The almost equal results obtained with the proposed Generalized Shvab-Zel'dovich model and the traditional Shvab-Zel'dovich model (Caldeira *et al.*, 2004) are observed in Fig. 3 and Fig. 4. This fact is explained, because the GSZ model is an extension of the traditional Shvab-Zel'dovich model. In other words, the same results are found, when unitary Lewis number cases are simulated in both models, considering the same physical and numerical conditions.

The unitary Lewis number case of infinite gaseous pocket array combustion with $b = 2$ was studied by Caldeira *et al.*, (2008). These results are compared with the GSZ ones in Fig. 5 and 6. The normalized mass of fuel and the flame behavior evolutions along of the time are, respectively, reported in Fig. 5 and 6. The physical conditions consider: $Le_f = 1$, $Le_o = 1$, $Pe = 1$, $s = 0.25$, $q = 2$, $b = 2$ and the initial fuel temperature equal to 10% of the initial oxidant temperature. Inert chemical species are not considered. The hybrid mesh with 115×70 volumes is employed in this simulation. The numerical solution was stopped when the fuel mass in the system was 2.5% of the initial mass of fuel (Caldeira *et al.*, 2004, 2008).

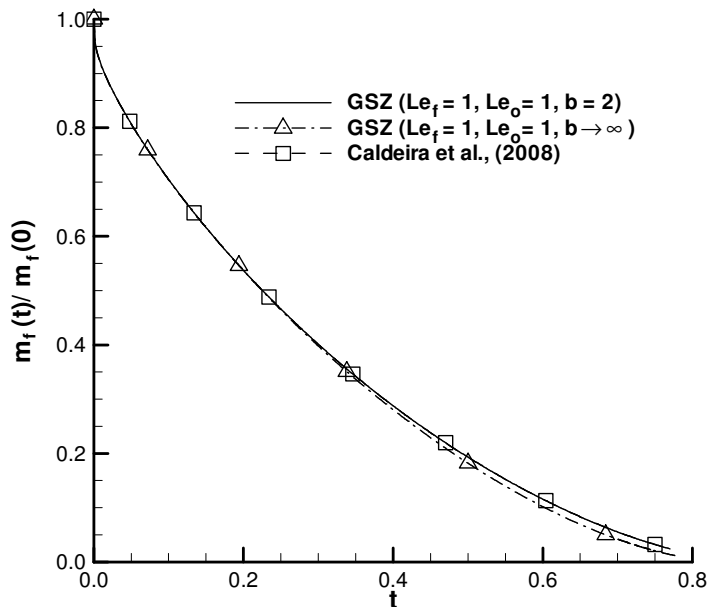


Figure 5. Normalized mass of fuel ($Le_f = 1$, $Le_o = 1$, $b = 2$).

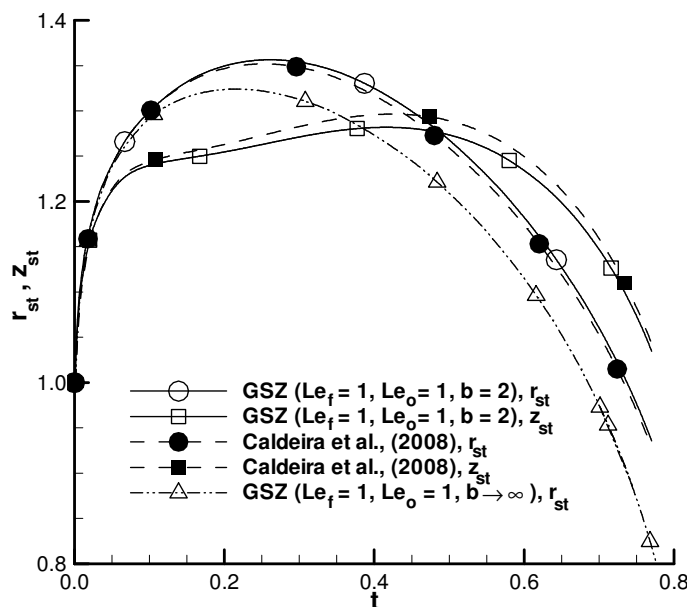


Figure 6. Flame behavior ($Le_f = 1$, $Le_o = 1$, $b = 2$).

Small differences between the results for $b = 2$ are observed in Fig. 6. These differences are minor than 0.4% and 2% for the flame position, respectively, on the equatorial pocket plane and on the array axis.

The congruence of the curves for gaseous pocket array combustion in Fig. 5 and in Fig. 6 indicate that, in interactive gas pocket conditions, the solutions obtained with the GSZ model for the unitary Lewis number case and the traditional Shvab-Zel'dovich model (Caldeira *et al.*, 2008) are consistent with the theory.

In Fig. 5 and 6 the results obtained with the proposed model for the isolated gas pocket combustion are also shown. Then, the half-interpocket distance effects on the combustion process can be analyzed. In Fig. 5, there is a small difference between the studied half-interpocket cases at the end of the combustion process. It reveals that the

combustion lifetime increases when the half-interpocket distance is reduced. In Fig. 6 there are strong differences in the flame behavior between isolated and array combustion. In $b = 2$ curves, the flame deforms from spherical ($r_{st} = z_{st}$) to an elliptical shape ($r_{st} \neq z_{st}$). In the elliptical regime, the flame have, initially, the major axis aligned with the pocket equatorial plane ($r_{st} > z_{st}$), but as the fuel amount is reduced in the system, the flame stand-off is also reduced and the flame recovers the spherical shape ($r_{st} = z_{st}$). Intensifying this process, the flame reaches an elliptical shape with major axis aligned with the array axis ($r_{st} < z_{st}$). Furthermore, the maximum stand-off in the equatorial pocket plane is greater in the $b = 2$ case than in the isolated gas pocket case. The proximity of the pockets changes the fluid dynamics reducing the velocity in the array axis direction and increasing the velocity in the equatorial pocket plane. It modifies the reactants mass flux to the flame. In the interpocket region, each pocket pair furnishes fuel to the flame, consuming oxidant faster than in the other regions.

The results obtained with the GSZ model are shown in Figs. 7-10 for nonunitary Lewis number cases, considering the isolated gas pocket condition. In these figures, the unitary Lewis number curves described in Fig. 3 and 4 are also plotted for comparison purposes.

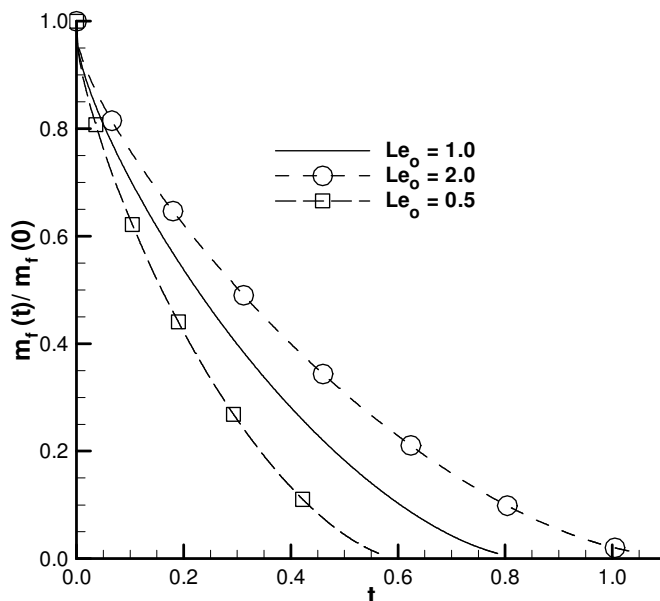


Figure 7. Normalized mass of fuel with nonunitary Lewis number ($b \rightarrow \infty, Le_f = 1$).

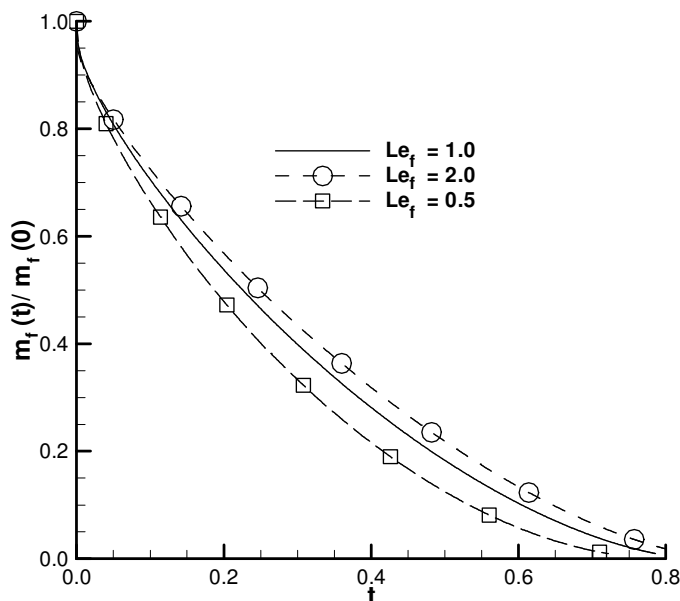


Figure 8. Normalized mass of fuel with nonunitary Lewis number ($b \rightarrow \infty, Le_o = 1$).

The normalized mass of fuel evolution along of the time could be observed in Fig. 7 and 8. The reduction of the Lewis number of the reactants decreases the burning time. Otherwise, increasing the Lewis number of the reactants, the

burning time is also increased. The same analysis can be done with relation to the fuel consumption which is proportional to the inclination of the curves plotted in Fig. 7 and 8. The reduction of the Lewis number of the reactants improves the diffusive mass flux of reactants to the flame, increasing the fuel consumption.

The flame behavior for isolated gas pocket with nonunitary Lewis number is reported in Fig. 9 and 10. In isolated gas pocket condition the r_{st} and the z_{st} are equal. So, the r_{st} variable is used to represent the flame evolution along of the time.

In Fig. 9, increasing the Lewis number of the oxidant, the flame stand-off is also increased and diminishing the Lewis number of the reactants, the flame stand-off decreases. This process is controlled by the mass flux of oxidant to the flame. When the mass diffusivity is improved, the flame stand-off is reduced. The same behavior was just reported with relation to oxidant diffusivity, “[...] increasing the diffusion coefficient of the oxidizer (decreasing oxidizer Lewis number Le_o) [...] reduces both maximum flame radius and nondimensional burning time, by bringing the oxidizer more rapidly to the flame” (Fachini *et al.*, 1999).

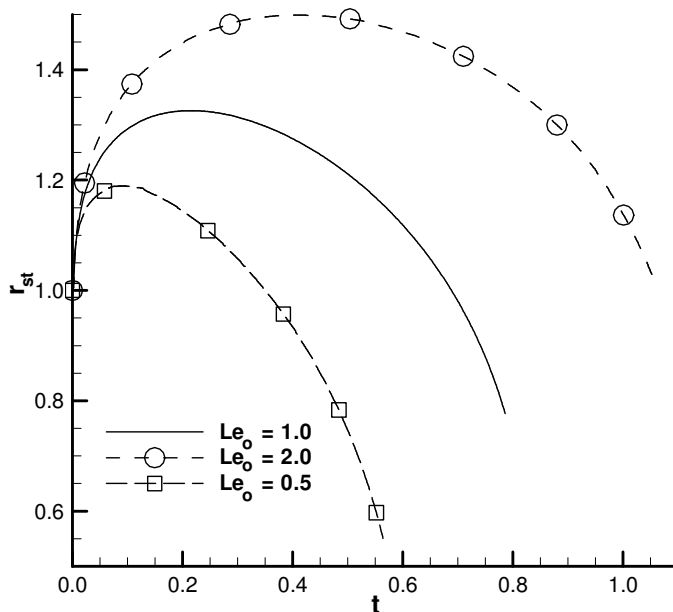


Figure 9. Flame behavior with nonunitary Lewis number ($b \rightarrow \infty, Le_f = 1$).

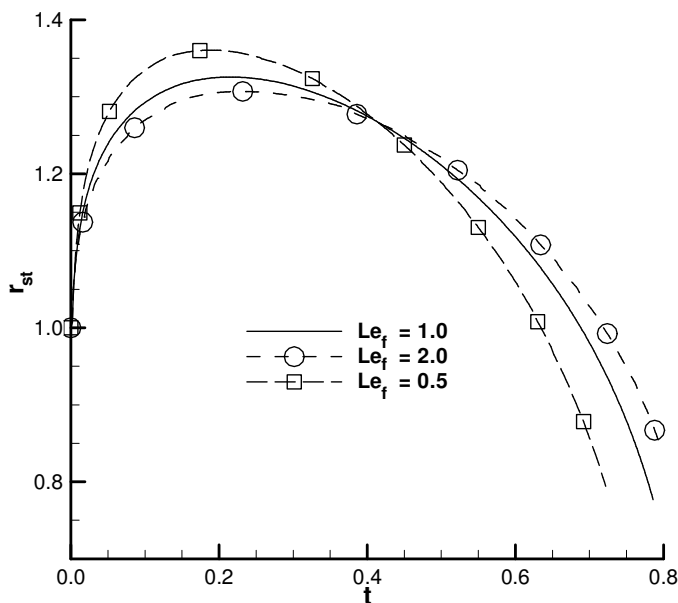


Figure 10. Flame behavior with nonunitary Lewis number ($b \rightarrow \infty, Le_o = 1$).

In Fig. 10, increasing the Lewis number of the fuel, the flame stand-off is reduced and diminishing the Lewis number of the fuel, the flame stand-off increases. This process is also controlled by the mass flux of fuel to the flame. When the mass diffusivity is improved, the flame stand-off is also improved. However, a different behavior can be

observed in Fig. 10. The flame curves for nonunitary Lewis number cross the flame curve for unitary Lewis number. It is not observed for nonunitary oxidant Lewis number cases in Fig. 9. So, for $Le_f = 0.5$, the more intense fuel mass flux in the initial times of the burning process pushes the flame far from the pocket center. Under this condition the fuel consumption is increased, reducing the pocket lifetime. Then, after the maximum flame stand-off, the flame moves fast to the pocket center. Otherwise, $Le_f = 2.0$, the fuel mass flux, the fuel consumption and the maximum flame stand-off are reduced, improving the pocket lifetime and resulting in a slow movement of the flame to the pocket center. These phenomena are also observed by Fachini *et al.*, (1999). The pocket has a limited capacity to furnish fuel to the flame, but the oxidant environment has an unlimited capacity to supply the chemical reaction.

From Fig. 7-10, it is verified that the effects of the oxidant Lewis number on the fuel consumption and on the flame behavior are more relevant than the effects of the fuel Lewis number.

5. CONCLUSIONS

The unitary Lewis number cases studied in the present work for isolated gas pocket and interactive gas pocket array are relevant to verify the quality of the proposed model and the numerical solution. The results obtained with the proposed model for unitary Lewis number are compatible with the results obtained with the traditional Shvab-Zel'dovich model. It is expected since the GSZ model is an extension of the traditional Shvab-Zel'dovich model.

The nonunitary Lewis numbers are evaluated for the isolated gas pocket combustion. This special condition is important to analyze the influence of the nonunitary Lewis numbers on the flame dynamics without interactive gas pocket effects. The effects of the nonunitary Lewis number on the flame behavior and on the fuel consumption are in agreement with the reference work (Fachini *et al.*, 1999). The results show that the flame stand-off and the burning time are controlled by the reactants mass flux to the flame. Then, improving the oxidant mass flux the flame stand-off is reduced. Otherwise, improving the fuel mass flux the maximum flame stand-off increases. Moreover, the influence of the oxidant Lewis number on the flame behavior is more effective than the fuel Lewis number.

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