ON THE COMBUSTION OF LINEAR STREAMS OF DENSE GAS POCKETS

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1 Introduction

Supercritical droplet combustion is present in a wide variety of engineering systems, such as Diesel, rocket and gas turbines engines. In these systems, the liquid droplets are injected into a supercritical environment and the droplets rapidly reach supercritical conditions. In the absence of a sharp liquid-vapor interface, of surface tension and of vaporization enthalpy effects, a supercritical droplet behaves as a dense gas pocket [1]. Reviews on supercritical droplet combustion indicate the absence of reliable experimental data [2], rendering importance to numerical modeling studies.

The numerical solution of the combustion of an infinite stream of dense gas pockets is described in the present work. The Finite Volume Method is employed for the numerical solution of the governing equations using a generalized system of coordinates formulation associated with hybrid grid generation techniques [3]. The SIMPLEC algorithm on a non-staggered grid is applied for the solution of the modified pressure-velocity coupling. In order to validate the developed numerical solution, results for the limiting case of an isolated pocket are compared with benchmark results available in the literature.

2 Analysis

The combustion of an infinity stream of initially spherical supercritical dense fuel gas pockets under microgravity conditions is studied considering temperature-only dependent density. The remaining thermo-physical properties are assumed invariant during the processes. The system is considered isobaric and the Simple Chemical Reaction mechanism is also applied. The mathematical model is based on the mass, momentum, energy and species conservation equations and on the ideal gas equation of state [1]. Initially, a stream of spherical, monosized and equidistant fuel pockets is assumed inside a stagnant oxidant atmosphere. Inside the pockets, temperature is uniform and below the constant environment temperature.

The solution domain, as depicted in Fig.1, is simplified exploring symmetries of the phenomena. In nondimensional and conservative form, the conservation equations are written in the spherical coordinated system (R, θ) positioned at the pocket center, as shown in the Fig.1, as

$$\frac{\partial \left(R^2 \sin \theta \rho\right)}{\partial t} + \frac{\partial \left(R^2 \sin \theta \rho u\right)}{\partial R} + \frac{\partial \left(R \sin \theta \rho v\right)}{\partial \theta} = 0 \tag{1}$$

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Fig. 1 – Sketch of the physical (left) and simplified domain (right).

$$\frac{\partial \left(R^{2} \sin \theta \rho u\right)}{\partial t} + \frac{\partial \left(R^{2} \sin \theta \rho u u\right)}{\partial R} + \frac{\partial \left(R \sin \theta \rho v u\right)}{\partial \theta} - \rho v^{2} R \sin \theta =$$

$$- R^{2} \sin \theta \frac{\partial p}{\partial R} + \frac{\partial}{\partial R} \left(R^{2} \sin \theta \tau_{RR}\right) + \frac{\partial}{\partial \theta} \left(R \sin \theta \tau_{R\theta}\right) - R \sin \theta \left(\tau_{\theta\theta} + \tau_{\varphi\varphi}\right)$$

$$\frac{\partial \left(R^{2} \sin \theta \rho v\right)}{\partial t} + \frac{\partial \left(R^{2} \sin \theta \rho u v\right)}{\partial R} + \frac{\partial \left(R \sin \theta \rho v v\right)}{\partial \theta} + \rho u v R \sin \theta =$$

$$- R \sin \theta \frac{\partial p}{\partial \theta} + \frac{\partial}{\partial R} \left(R^{2} \sin \theta \tau_{R\theta}\right) + \frac{\partial}{\partial \theta} \left(R \sin \theta \tau_{\theta\theta}\right) + R \sin \theta \left(\tau_{R\theta} - \cot g \theta \tau_{\varphi\varphi}\right)$$
(2)
(3)

$$\frac{\partial \left(R^2 \sin\theta \rho f\right)}{\partial t} + \frac{\partial \left(R^2 \sin\theta \rho u f\right)}{\partial R} + \frac{\partial \left(R \sin\theta \rho v f\right)}{\partial \theta} = \frac{\partial}{\partial R} \left(\frac{R^2 \sin\theta}{Pe} \frac{\partial f}{\partial R}\right) + \frac{\partial}{\partial \theta} \left(\frac{\sin\theta}{Pe} \frac{\partial f}{\partial \theta}\right)$$
(4)

where

$$\tau_{RR} = \frac{2}{Re} \frac{\partial u}{\partial R}, \ \tau_{\theta\theta} = \frac{2}{RRe} \left(\frac{\partial v}{\partial \theta} + u \right), \ \tau_{\varphi\varphi} = \frac{2}{RRe} \left(u + v \cot g \theta \right), \ \tau_{R\theta} = \frac{1}{Re} \left(\frac{\partial v}{\partial R} - \frac{v}{R} + \frac{1}{R} \frac{\partial u}{\partial \theta} \right)$$
(5)

and p represents a modified pressure, which accounts for the thermodynamic pressure and the volumetric expansion terms [1]. Density (ρ) values are related to mixture fraction (f) through the equation of state written as

$$\rho = \begin{cases} \left[l - (l - e) f + q f \right]^{-l}, f \le f_{st} \\ \left[l - (l - e) f + q f_{st} \frac{(l - f)}{(l - f_{st})} \right]^{-l}, f \ge f_{st} \end{cases}$$
(6)

where f_{st} is the stoichiometric mixture fraction coefficient, *e* is the initial pocket to ambient temperature ratio and *q* is the heat of reaction.

The initial gas pocket radius (R_0^+) is used as the characteristic length. The characteristic velocity $(\rho_{\infty}^+ R_0^+ / \mu_{\infty}^+)$ is based on a diffusive scale. Therefore, the Reynolds number becomes equal to 1 and the Peclet number is equal to the Prandlt number evaluated in the undisturbed environment conditions.

The initial mixture fraction distribution is f = 1 within the fuel pocket and f = 0 in the oxidizing environment. Homogeneous Von Neumann boundary conditions are used for each dependent variable. These boundary conditions are based on the symmetries of the problem and on the undisturbed condition along the truncation boundary as $r + \rightarrow \infty$, which can be noted in Fig.1.

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3 Numerical Solution

The conservation equations (Eqs. 1-4) are transformed into a generalized coordinated system (ξ,η) . The domain is divided into three subregions. The discretization procedure uses a combination of numerical and analytical grid generation techniques. The mesh generation explores physical aspects of the problem of the infinity stream of point sources [4], since the η -grid lines are similar to the streamlines emerging from the dense pocket. The numerical procedure also uses a double-grid procedure [3] where the volumes and their faces are represented by grid points. This procedure improves the precision of the flux evaluation, since the transformation metrics are also computed at the volumes faces.

The Finite Volume Method is employed using a non-staggered grid and the SIMPLEC algorithm is applied to address the modified pressure-velocity coupling. WUDS is used as the interpolation function in an implicit scheme. The resulting system of linear of algebraic equations is solved by the GMRES algorithm. The computational procedure is validated using limiting case results with analytical solutions. The consistency of the numerical results is also evaluated [3]. In the present work, a mesh with 3200 volumes is used for the isolated pocket $(b \rightarrow \infty)$ combustion case. For the interacting cases with b = 4 and b = 2, 11664 and 10944 volumes are employed, respectively.

Once converged profiles are obtained for a given time moment, the fuel mass within the solution domain is evaluated by

$$m_F(t) = \iint_{V_{st}} \left\{ \left(\frac{f - f_{st}}{1 - f_{st}} \right) \rho \right\} dV$$
(8)

where V_{st} is the volume enclosed by the isopotential surface f_{st} , that represents the reaction sheet, and the solution domain boundaries.

4 Results

Initially, a parametric study is conducted using the data from the work of Daou and Rogg on an isolated deforming pocket [1] to establish a reference case with e = 0.1, q = 2, $f_{st} = 0.8$, Pe = 1 and b = 2.

A parametric study based on the fuel mass temporal evolution for b = 2 is shown in Fig. 2. Reference case results are also depicted in Fig.2. Results show that increasing the initial temperature ratio (e) to 0.2, the pocket lifetime is reduced by 50% when compared with the reference case (e = 0.1). The increase of e leads to a reduction on the initial fuel mass within the domain that explains the observed reduction in the pocket lifetime.

The effect of the amount of heat released by the chemical reaction is also depicted in Fig. 2. For early times (t < 0.45), the results for fuel mass within the solution domain without heat release are smaller than to reference case values (q = 2), indicating a higher fuel consumption rate for q = 0. The results in Fig. 2 show that reducing the heat release from 2 to zero the burning time is increased by 20%. The nonvanishing heat release (q) leads to thermal expansion effects that increase the local flame standoff distance during the initial stages of the combustion process. By altering the fuel concentration gradients, thermal expansion reduces diffusional mass transfer to the flame. As density gradients evolve and thermal expansion effects weaken, heat and mass transfer increases the fuel consumption for the heat release case near the end of the combustion process.

The stoichiometric mass fraction (f_{st}) defines the flame sheet locus within the mass fraction field. As the mixture fraction parameter (f_{st}) is reduced, more oxidant is required by a given amount of fuel leading to an increase of the flame stand off distance. Results in Fig. 2 depict this behavior indicating an increase of 352% in the burning time as f_{st} is reduced from 0.8 to 0.2.

Reducing the Peclet number, the thermal and the mass diffusivities increase as a result of the unitary Reynolds and Lewis numbers. In consequence, energy and mass transfer processes are enhanced leading to reduction on the burning time as shown in Fig. 2. Results depicted in Fig.2 show that as Pe is reduced from 1 to 0.5 the burning time is reduced by 50%.

A parametric study is also performed for the temporal evolution of the flame position along a pocket equatorial plane (r_{st}) and the stream axis (z_{st}) for b = 2. Results are depicted in Fig.3, showing that flame positions are affected by variations on the studied parameters $(e, q, f_{st} \text{ and } Pe)$. For all studied cases, the flame initially moves away from the pocket, experimenting deformation due to interference effects. After reaching a maximum distance from the droplet stream along the pocket equatorial plane, the flame recedes towards the pocket center. For the nonexothermic cases (q = 0), the maximum standoff position along the pocket equatorial plane $(r_{st} = 1.02)$ is slightly higher than the initial pocket surface position $(r_{st} = 1)$. For all studied cases, fuel and the oxidant mass fraction fields control the flame displacement. The flame moves towards regions with higher fuel concentration. These transient flame behaviors are also described for subcritical and supercritical droplet combustion [4] and for the combustion of gas clouds [2].

Results obtained for different interpocket distances show small variations in pocket lifetime for $b \rightarrow \infty$ and b = 4. Nevertheless, an increase of 3.5% in the burning time for the reference case (b = 2) is found in relation to the non-interacting cases. Through the temporal evolution of the flame position along the equatorial gas pocket plane (r_{st}) and the gas pocket-stream axis (z_{st}) , the flame deformation process due to interference effects is identifiable showing the existence of the four flame morphologies. Numerical results also allow the study of the temporal evolution of the dense gas pocket shape. Due to the absence of a sharp liquid-gas interface, the pocket boundary is arbitrarily defined in the present work as the locus where fuel mass fraction is equal to 99%.



Figure 2. Normalized fuel mass along of the time, parametric analysis for b = 2.



Figure 3. Flame position on the equatorial droplet plane (r_{st}) and on droplet-stream axis (z_{st}) , parametric analysis for b = 2.

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