Detailed Numerical Simulation of the Extinction of Lean Premixed Flames Through Parallel Plates

Luigi Tecce[1], Francesco Saverio Marra[2] and Gaetano Continillo[1]
[1]Department of Engineering, Università del Sannio, Benevento, Italy
[2]Istituto di Ricerche sulla Combustione CNR, Naples, Italy

Corresponding author, G. Continillo: continillo@unisannio.it

Introduction

This work attempts to reproduce experimental results (Mihalik *et al*, 2000) and understand predominant extinction mechanisms. Simulations are conducted as the flame approaches parallel plates in a tube as shown in Fig 1. Two–dimensional simulation flame propagation at near–extinction conditions are conducted with CFD-ACE (CFDRC, 2003). The computational domain is discretised by means of a structured mesh with over 23,000 nodes. Evaluation of heat fluxes and strain rate for three cases are considered: “real”, “adiabatic” and “free–slip” at the plate boundaries, to elucidate the mechanism of flame extinction.

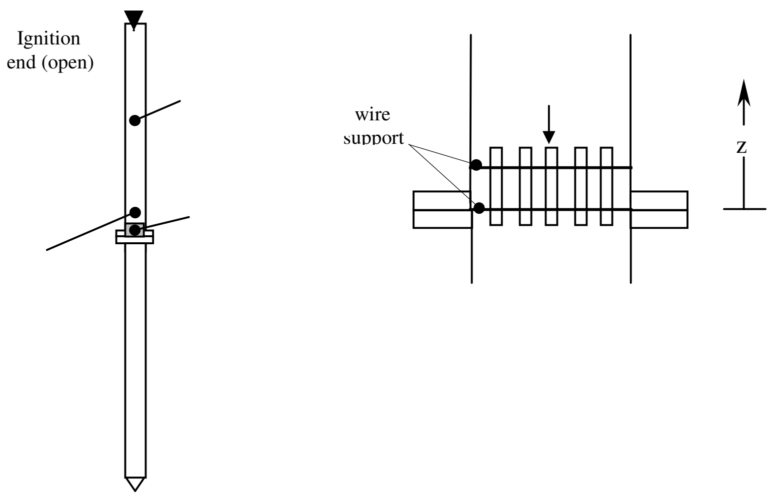

Figure 1. Schematic of the experimental apparatus used in Mihalik *et al*, 2000.

Numerical model

To simulate the flame impact with the parallel plates without having to develop a three–dimensional model, planar symmetry is assumed for all single plates. Model equations correspond to full Navier–Stokes for reactive flows, in the limit of low Mach number. Neglecting Soret and Dufour effects, the equations are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0$$

$$\frac{\partial}{\partial t}\rho_k = -\nabla \cdot \left(\rho_k \mathbf{v} + \mathbf{j}_k\right) + r_k \qquad k = 1,\dots,N$$

$$\frac{\partial}{\partial t}\rho \mathbf{v} = -\nabla \cdot \rho \mathbf{v}\mathbf{v} - \nabla p + \nabla \cdot 2\mu \left(\nabla \mathbf{v}\right)_0^S + \rho \mathbf{g}$$

$$\frac{\partial}{\partial t}\left[\rho\left(u+\frac{1}{2}v^2\right)\right]=-\nabla\cdot\left[\rho\left(u+\frac{1}{2}v^2\right)\mathbf{v}+\mathbf{q}+p\mathbf{v}-2\mu\left(\nabla\mathbf{v}\right)_0^S\cdot\mathbf{v}\right]+\rho\mathbf{v}\cdot\mathbf{g}$$

$$p=\rho\left[\left(\sum_{k=1}^{N}\frac{y_k}{W_k}\right)R_0\right]T=\rho RT$$

The reaction is one–step with Arrhenius dependence on the temperature. The expression for the reaction rate for species *k* with stoichiometric coefficient ν_k is:

$$r_k=-W_k\nu_k AT^f\exp\frac{E}{R_0T}\rho^\gamma\prod_j y_j^{\beta_j}$$

In the above formulae symbols denote respectively: ρ: density, μ: viscosity, $\mathbf{v}$: velocity, p: pressure, T: gas temperature, u: internal energy, $\mathbf{q}$: conduction heat flux, $\mathbf{g}$: gravity, R_0: universal gas constant; ρ_k, J_k, y_k, W_k, and r_k: partial density, mass diffusion flux, mass fraction, molecular weight and reaction rate of species *k*. Here $2\mu\left(\nabla\mathbf{v}\right)_0^S$ is the null-trace symmetric stress tensor. Radiation heat flux is neglected as usually done in the literature. It may become significant with rich mixtures and luminous sooty flames at high temperatures: in this latter case, radiation heat flux to the duct walls might not be neglected even for weak flames at the rich extinction limit (Sorhab and Law, 1984). The study is limited to lean mixtures with no soot. Since the aim of this study is a detailed evaluation of the various contributions to heat losses, special attention has been devoted to molecular heat and mass transfer. Indeed it is known that the quenching distance depends on the Lewis number of the mixture (Sato *et al*, 1982, Kurdyumov *et al*, 2002). Moreover, the influence of preferential diffusion depends quantitatively on the direction of flame propagation with respect to gravity (Jarosinski et al 2002) To evaluate mass diffusivities, the classic Chapman–Enskog law for low-density gases is employed. The non–dimensional parameter related to molecular transport phenomena is obviously the Lewis number that, for species *k*, is: $\mathrm{Le}_k=\lambda/\rho C_p D_k$. Parameters of the chemical reaction rate were taken from (Westbrook and Dryer). The pre-exponential factor of this global kinetic model was lowered to ensure quantitative agreement on the lean extinction limit for downward propane–air flame propagation, and kept unchanged thereafter. Analysis of flame stretch is done through the evaluation of the Karlovitz number, defined as $\mathrm{Ka}=K\,\delta/S_L$, representing the influence of strain on flame extinction. Here δ indicates the flame thickness, S_L the laminar flame speed, and K is the following quantity: $K=\sqrt{S_{11}^2+S_{22}^2+2S_{12}S_{21}}$, with $S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$.

Results and discussion

Here we report the flame behaviour at the impact with the array of plates for the three different boundary conditions: "real", adiabatic and free–slip. Plate material was chosen as steel: however, as expected, its thermal properties have no influence on the results. Figure 2 shows a comparison of the three cases in terms of flame location versus time. All flames propagate in a very similar manner until the channel entrance is reached after about 0.15 s. The "adiabatic" case sees the flame propagate throughout the tube, while the "free-slip" case (minimal deformation of the flow) sees flame extinction with little if any quantitative differences with respect to the "real" case, in which flow deformation due to viscous wall effects is regularly taken into account.

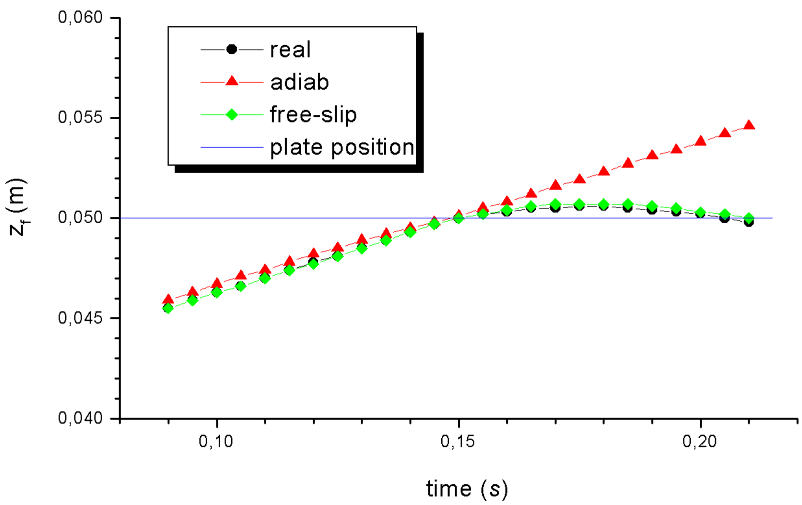

Figure 2. Flame location vs time for the three cases.

Figure 2 reports reaction rate contours to indicate flame shape and location at a single time snapshot, at the impact of the flame with the plate rim. The picture at the centre (adiabatic case) shows the flame progressed well inside the plate array (no extinction), while the one at left ("real") shows the flame "standing" outside, where it will eventually extinguish. Comparison between "real" and adiabatic indicates the key role of heat transfer to the plates. The rightmost picture (free–slip) shows little change with respect to the "real", thus indicating a minor influence of the strain.

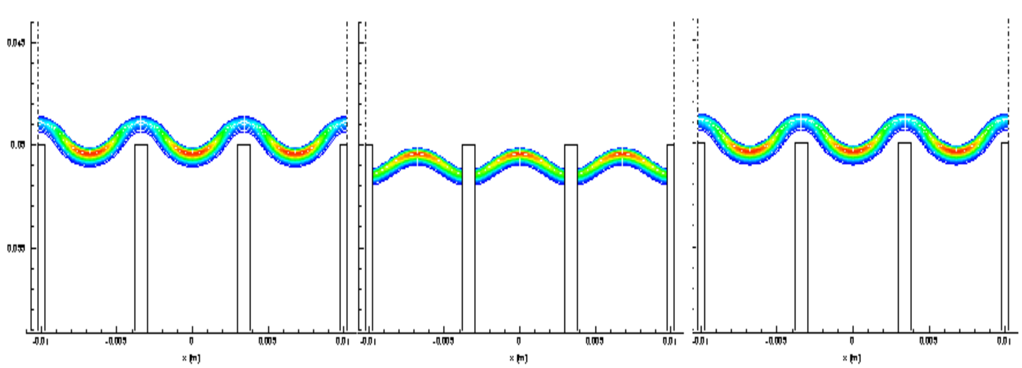

Figure 3. Reaction rate contours showing flame shape and location for the three cases ("real", adiabatic and free–slip) at $t = 0.16$ s.

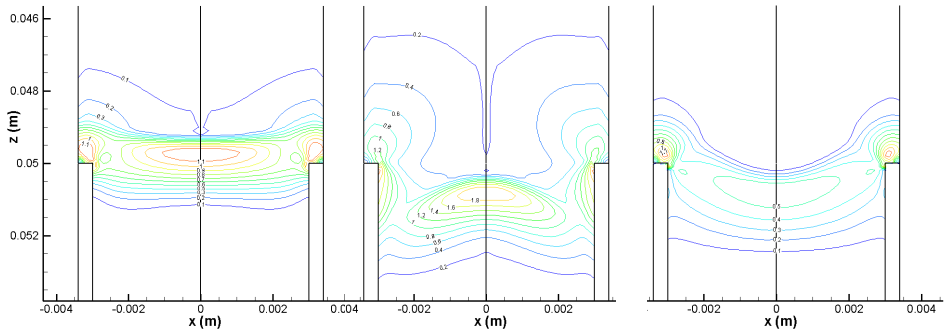

Figure 4. Karlovitz number contours close to the plates for three cases ("real", adiabatic and free–slip) at $t = 0.16$ s.

Figure 4 reports the distribution of the Karlowitz number at t=0.16 s for the three cases ("real", adiabatic and free-slip). It is found that the Karlowitz number achieves its maximum value (about 2) in the "adiabatic" (successful propagation) case, and never near the flame region. In contrast, the "free-slip" simulation, conducted to test the system at minimum flow deformation conditions, leads to flame extinction even though the Karlowitz number remains very small everywhere in the system. This confirms that flame stretch does not play a role in flame extinction under the present circumstances.

All reported results indicate that heat transfer to the wall is the main mechanism leading to extinction.

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