Numerical study of the propagation of lean hydrogen-air flames in Hele-Shaw cells

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Introduction

The premixed propagation of lean hydrogen-air flames ($\phi = 0.3$) in Hele-Shaw cells (i.e. two adiabatic parallel plates separated by a small distance h [1–3]) is investigated using numerical simulations with detailed chemistry and transport. We focus on the effect of the distance between plates, h, for a semi-closed system of size $50\delta_f \times 50\delta_f \times h$, where $\delta_f = 3.45$ mm is the thickness of the planar adiabatic flame. Hydrodynamic and diffusive-thermal instabilities wrinkle the flame front to form small cellular structures that increase the overall propagation velocity. Symmetric and non- symmetric shapes are observed in the third dimension (i.e. along h).

Formulation

The dynamics of the flame front is determined by solving the variable-density reactive Navier-Stokes equations:

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

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla\cdot(\rho \mathbf{v}\cdot\mathbf{v}) = -\nabla p + \nabla\cdot\tau,$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla\cdot(\rho \mathbf{v} Y_k) = -\nabla\cdot\mathbf{j}_{\mathrm{k}} + \dot\omega_k,$$

$$\frac{\partial}{\partial t}(\rho h_s) + \nabla\cdot(\rho \mathbf{v} h_s) = -\nabla\cdot\mathbf{j}_{\mathrm{q}} - \sum_{k=1}^{N-1}\Delta h_{f_k}\dot\omega_k,$$

with the ideal gas equation of state:

$$\rho R_g T = p.$$

The species flux and the heat flux have the form $\mathbf{j}_{\mathrm{k}} = \rho\,\mathcal{D}_{k,m}\nabla Y_k$ and $\mathbf{j}_{\mathrm{q}} = -\lambda/c_p\left(\nabla h_s - \sum_{k=1}^{N-1} h_{s_k}\nabla Y_k\right) + \sum_{k=1}^{N-1}\mathbf{j}_{\mathrm{k}} h_{s_k}$, respectively. The diffusivity of the species into the mixture $\mathcal{D}_{k,m}$ is calculated using mixture-averaged diffusion model. The chemistry is modeled using the Mével's mechanism for hydrogen oxidation, which includes $N = 9$ species and 21 reactions [4]. A detailed comparison of the ignition delay time and flame speed performance of Mével's mechanism with others commonly used in the literature is provided in [5, 6].

Results

The mixture is ignited at the open-to-atmosphere end ($x = 0$ cm) with a series of evently-spaced hot spots. The reactive front propagates towards the closed end ($x = 17.25$ cm). The simulations compare three cases: $h = 0.1\delta_f$, $h = \delta_f$ and $h = 3\delta_f$ at $t = 0.14$, 0.31 and 0.06 seconds from the initial ignition, respectively.

Diffusive-thermal instabilities (associated with the small effective Lewis number of these mixtures, $Le_{\mathrm{eff}} \approx 0.3$) promote chaotic cell splitting and merging observed along y in all the simulations. In Fig. 1, for $h = 0.1\delta_f$, the gap is so tight (smaller than the critical wavelength for instability) that only planar flame structures can be seen in the third dimension. For this case, the corresponding three-dimensional problem can be reduced to a two-dimensional set of equations governed by Darcy's law (i.e. narrow-channel approximation [7]).

For $h = \delta_f$ the narrow-channel approximation breaks down. We show in Fig. 2 the emergence of non-symmetric shapes in the third dimension, similar to those observed in [8], which increase the total flame surface area. Fig. 3 depicts a symmetric V-shape flame that appears during the early stages of the flame evolution for $h = 3\delta_f$.

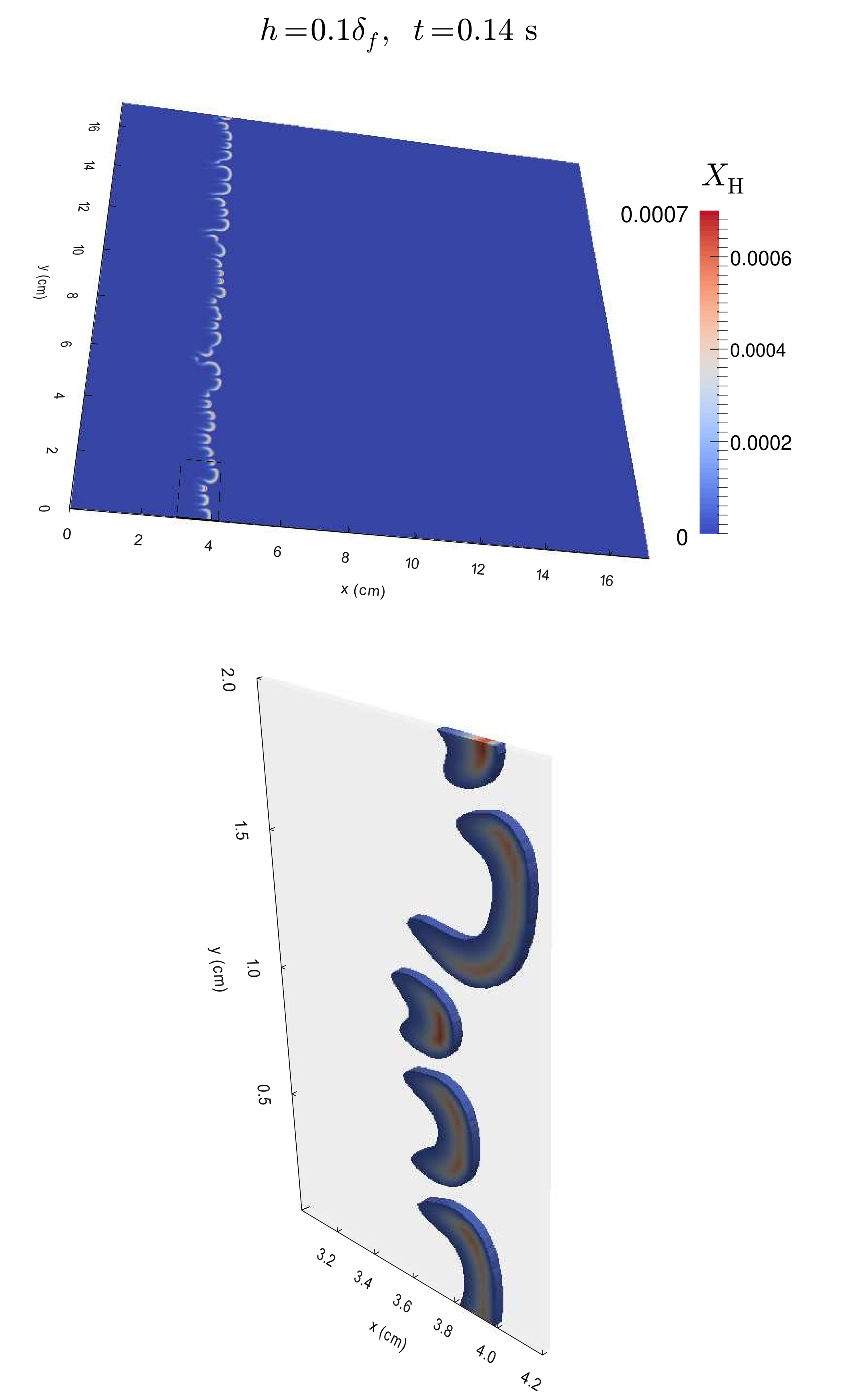

Fig. 1: Field of H-mole fraction for $h = 0.1\delta_f$ showing the flame front curvature at time $t = 0.14$ s. Flame propagates from left to right.

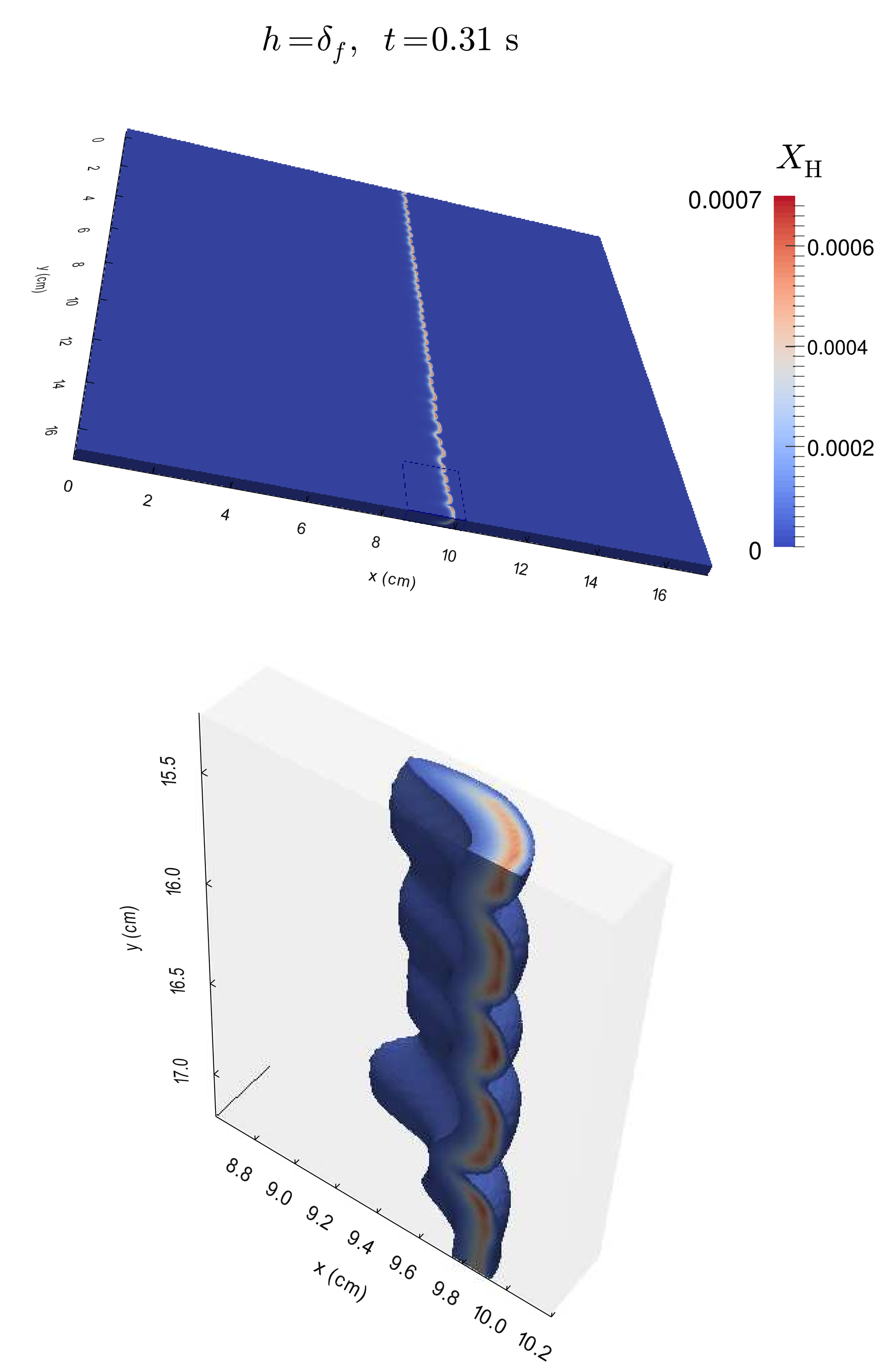

Fig. 2: Field of H-mole fraction for $h = \delta_f$ showing the flame front curvature at time $t = 0.31$ s. Flame propagates from left to right.

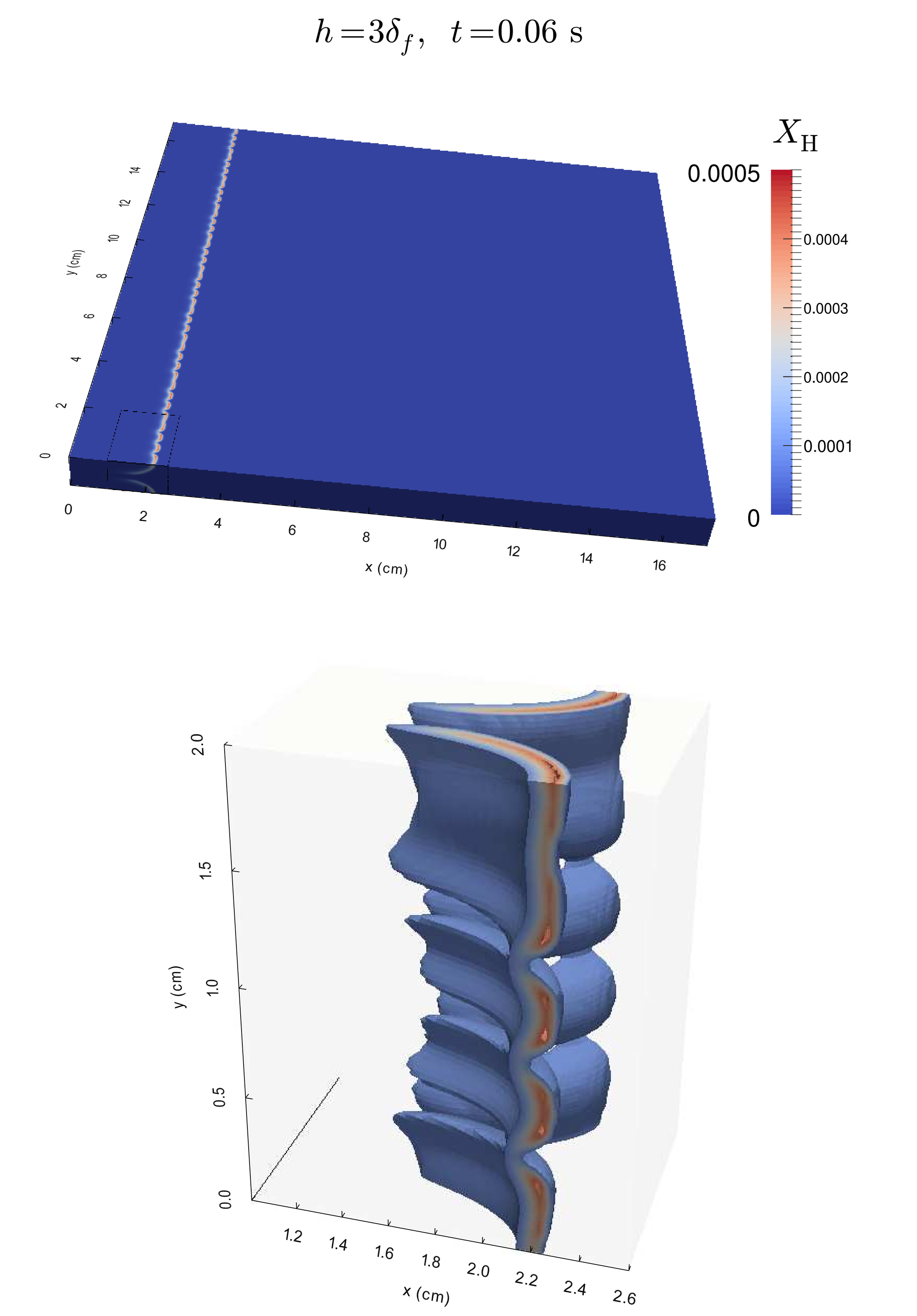

Fig. 3: Field of H-mole fraction for $h = 3\delta_f$ showing the flame front curvature at time $t = 0.06$ s. Flame propagates from left to right.

Work in progress

Long-time flame evolution will be investigated by implementing the formulation in a reference frame moving with the flame. The velocity of this reference frame can be calculated from $\iiint \dot\omega_{\mathrm{H}_2}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z/(\rho_u Y_{\mathrm{H}_{2u}} S_L h L_y)$.

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