Suppression of instabilities in a premixed methane–air flame in a narrow channel via hydrogen/carbon monoxide addition

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ABSTRACT

The effects of hydrogen and carbon monoxide addition on premixed methane/air flame dynamics in a heated narrow channel are numerically investigated using a time accurate, compressible flow solver along with the DRM-19 reaction mechanism. By adding a small amount of either H_2 or CO, flame instabilities present for the pure CH_4/air combustion in the form of flame-extinction and re-ignition could be effectively suppressed. This suppression can be attributed to a few important elementary reactions, that play a dominant role in contributing to the heat release rate, getting enhanced with H_2 or CO addition. This leads to a higher flame propagation speed and a shorter flame-extinction period, and eventually leads to flame stabilisation after a few cycles of spatial oscillations.

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1. Introduction

Hydrocarbons have considerably higher specific energy per unit mass compared to the traditional electrochemical batteries (45 vs 0.6 MJ/kg). This energy can be harnessed via combustion in the form of heat and converted to useful power. In order to achieve this, combustion in a narrow passage where the characteristic dimension is of the order of the flame thickness has received considerable attention in the past two decades and is termed microscale (dimension <1 mm) or mesoscale (dimension close to flame thickness) combustion [1–11]. The potential applications include portable power systems and propulsion systems for small scale rockets [12]. More recently, the concept of "heat recirculating burners" has also found discussion in future bio-fuelled engines for transportation [13]. However, as the dimension of the combustor decreases, stable combustion becomes quite challenging to achieve because the increased surface-area-to-volume ratio leads to significant heat losses from the combustor outer surface. Consequently, these heat losses can potentially induce flame instabilities (e.g. flames with repetitive extinction and ignition (FREI) [14,15] and various other flame patterns [16–18]) or even flame quenching. Therefore, it is critical to understand and tackle these flame instabilities in order to make microcombustion a viable technology.

Past studies on conventional-scale methane (CH_4)–air combustion have shown that the introduction of low levels of either hydrogen (H_2) [19,20] or carbon monoxide (CO) [21] could en-

hance the flame burning velocity and thus extend the flame stability limits. On a micro/mesoscale, the addition of H_2 to a premixed CH_4/air mixture was also adopted as an approach for flame stabilisation and was found to play a positive role in assisting flame ignition [22,23] and sustaining vital radicals for stable combustion [24], while the addition of CO into a CH_4/air micro-flame has drawn limited research interest. The previous studies mainly focused on the microcombustor performance with H_2 addition in terms of fuel conversion rates and combustor outer surface temperature. However, fundamental aspects of gas-phase hydrodynamics and chemical kinetics (flame dynamics) also need to be better understood for H_2/CO addition. Numerical simulations are capable of revealing such physical aspects of the problem that are hard to measure experimentally owing to the inherent difficulties in obtaining spatially resolved measurements on a small scale. Some past studies [23,24] simulating the H_2 addition flame used a steady-state model to capture the overall flame stability limits and combustor performance. These, owing to solving for steady state, were not able to capture the transient flame behaviours. Other studies where time accurate numerical simulations were performed, e.g. Pizza et al. [25] and Alipoor et al. [26] for H_2/air, Miyata et al. [27] for CH_4/air and Kurdyumov et al. [28,29] for constant-thermodynamic/transport property gases with an overall-step reaction model captured the flame dynamics involving various modes of flame oscillations.

In the present numerical study, we focus on suppression of flame dynamics of premixed CH_4/air combustion with H_2 and CO addition in a narrow channel using a time-accurate solver. The focus on methane is owing to it being the majority constituent of typical natural gas fuel. Physical insights for the observed flame

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dynamics suppression are provided via inspection of reaction rates of some critical elementary reactions and their impacts on heat release.

2. Numerical approach

As mentioned earlier, the premixed CH_4/air flame propagation in a two-dimensional, planar micro-channel is numerically studied using our in-house code Eilmer [30]. A cell-centered, finite volume method is employed for the discretisation of the governing compressible Navier–Stokes equations which are expressed in the integral form:

$$\frac{\partial}{\partial t} \int_V U dV = - \oint_S \left(\overline{F}_i - \overline{F}_v\right) \cdot \hat{n} \, dA + \int_V Q dV \, , \tag{1}$$

where V is the control volume and S is the bounding surface. The symbol $\hat{n}$ represents the outward-facing unit normal of the bounding surface. U, $\overline{F}_i$, $\overline{F}_v$ and Q are the conserved quantities, inviscid fluxes, viscous fluxes and source terms respectively.

A detailed description of the solver and governing equations is given in the article by Gollan and Jacobs [30]. The key governing equations are repeated here for completeness. For a two-dimensional model, the array of conserved quantities U can be written as a summation of density, x-momentum per volume, y-momentum per volume, total energy per volume and mass density of species s:

$$U = \begin{bmatrix} \rho \\ \rho u_x \\ \rho u_y \\ \rho E \\ \rho f_s \end{bmatrix} . \tag{2}$$

u_x and u_y are the Cartesian velocity components, E is the specific total energy of the gas mixture (a sum of the internal energy and kinetic energy: $E = e + \frac{1}{2}(u_x^2 + u_y^2)$) and f_s is the mass fraction of species s.

The inviscid fluxes $\overline{F}_i$ are expressed as

$$\overline{F}_i = \begin{bmatrix} \rho u_x \\ \rho u_x^2 + p \\ \rho u_y u_x \\ \rho E u_x + p u_x \\ \rho f_s u_x \end{bmatrix} \hat{i} + \begin{bmatrix} \rho u_y \\ \rho u_x u_y \\ \rho u_y^2 + p \\ \rho E u_y + p u_y \\ \rho f_s u_y \end{bmatrix} \hat{j}, \tag{3}$$

where p is the static pressure.

The viscous fluxes $\overline{F}_v$ are expressed as

$$\overline{F}_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{xx} u_x + \tau_{yx} u_y + q_x \\ J_{x,s} \end{bmatrix} \hat{i} + \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{xy} u_x + \tau_{yy} u_y + q_y \\ J_{y,s} \end{bmatrix} \hat{j} \, . \tag{4}$$

The viscous stresses are

$$\tau_{xx} = 2\mu \frac{\partial u_x}{\partial x} - \frac{2}{3}\mu \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{u_y}{y}\right) \, ,$$

$$\tau_{yy} = 2\mu \frac{\partial u_y}{\partial y} - \frac{2}{3}\mu \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{u_y}{y}\right) \, ,$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u_x}{dy} + \frac{\partial u_y}{dx}\right), \tag{5}$$

where μ is the dynamic viscosity of the gas mixture. The viscous heat fluxes are

$$q_x = k\frac{\partial T}{\partial x} + \sum_{s=\text{all}} J_{x,s} h_s \, ,$$

$$q_y = k\frac{\partial T}{\partial y} + \sum_{s=\text{all}} J_{y,s} h_s \, , \tag{6}$$

where k is the thermal conductivity of the gas mixture, T is the static temperature, J_x and J_y are the species mass diffusion fluxes and h_s is the standard enthalpy of formation of species s.

The vector of source term Q on the right-hand side of the governing equation can be written as

$$Q = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_s \end{bmatrix} , \tag{7}$$

where $\dot{\omega}_s$ is the production/loss rate of species s.

The evaluation of thermodynamic and transport properties for the component species used curve fits collated by McBride and Gordon [31] for their CEA2 program. The state for the gas mixture was then calculated based on a mass fraction weighted sum of individual species for thermodynamic properties and using Wilke's mixing rule [32] for transport properties.

Fick's law, using mixture-averaged diffusion coefficients [33] was implemented to evaluate the species mass diffusion. The mixture-averaged diffusivity of species s is expressed as

$$D_s = \frac{1 - X_s}{\sum_{i \neq s}^N (X_i/\mathcal{D}_{si})}, \tag{8}$$

where X_s and X_i are the mole fractions of species s and i respectively, N represents the total number of species in the mixture, $\mathcal{D}_{si}$ is the binary diffusion coefficient for the species pair s and i and can be calculated from GRI-Mech3.0 transport database [34] using the Chapman–Enskog relation [33]. A correction for calculated fluxes was performed in order to guarantee total mass conservation numerically [35]. The species mass diffusion fluxes are thereby expressed as

$$J_{x,s} = -\rho D_s \frac{\partial f_s}{\partial x} - f_s \sum_{i=\text{all}} \rho D_i \frac{\partial f_i}{\partial x},$$

$$J_{y,s} = -\rho D_s \frac{\partial f_s}{\partial y} - f_s \sum_{i=\text{all}} \rho D_i \frac{\partial f_i}{\partial y}. \tag{9}$$

This diffusion model has been proved to be accurate enough to predict the laminar burning velocity of premixed methane/air flame compared to the full multicomponent diffusion model [36]. It should be mentioned that the Soret effect was not taken into account in the diffusion model, since the error in burning velocities by neglecting this effect was only around 2% for CH_4/air flame as reported by Bongers et al. [36].

The solver uses operator splitting to sequentially update the flow properties due to fluid dynamics (inviscid and viscous fluxes) and then the changes due to chemistry (combustion reactions). Time-accurate and numerically stable solutions are obtained by using the explicit three-stage *Runge–Kutta* time-marching scheme and setting the *Courant–Friedrichs–Lewy* (CFL) number to 0.3 to choose the simulation time step (on the order of 10^{-9} s).

Figure 1 shows the full channel, 2D computational domain and boundary conditions used for the numerical model. The channel length (L) is 6 mm and channel height (H) is 600 μm. The inlet of the combustor was modelled using a mass flux boundary condition in which the gas total temperature ($T_0 = 300$ K), mass fractions of incoming species and a uniform mass flux ($\dot{m}$) across the boundary were specified. At the outlet, the pressure was set at atmospheric pressure while zero *Neumann* boundary conditions were imposed