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Numerical Simulations of Premixed Combustion in Narrow Channels

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Abstract

Flame propagation in a mesoscale channel between two parallel heated plates is studied using detailed chemical kinetics (DRM19 reaction mechanism) for premixed methane-air combustion. The problem is modelled by solving the two-dimensional, transient, full Navier-Stokes equations in our in-house code (Eilmer). The effects of the prescribed wall temperature on the flame propagation are investigated. Mesoscale-channel flames with interesting characteristics such as spatially stable flames and flames with repetitive extinction and ignition (FREI) are observed at different wall temperatures.

Introduction

Mesoscale-combustion which can be viewed as combustion in narrow passages or ducts typically on the order of 1 mm finds application in portable power systems and propulsion systems for small scale rockets. As the combustor size decreases, the inherent gas-structure thermal coupling provides an additional mode of heat transfer that can either aid or retard the flame [1]. A detailed account of various studies in the experimental, theoretical and demonstrative realms can be found in recent comprehensive review articles [2,3].

Past work on experimental micro-combustion [4-8] established operational regimes/stability limits [4,5], investigated ability to make fundamental temperature and species concentration measurements in simulated micro-combustors [6] as well as demonstrated a range of interesting flame features such as flames with repetitive extinction and ignition (FREI) [7] and various flame patterns [8]. Correspondingly, theoretical modelling of micro-combustors has undergone rapid advances: simplified first-principles well-stirred reactor model for a counter-current combustor with heat recirculation by Ronney [9]; 1-D thermal resistance model based on flame thickness by Leach and Cadou [10]; 1-D quasi-steady model by Ju and Xu [11]; and 2-D conjugate heat transfer model by Veeraragavan and Cadou [12]. The theoretical models predict flame stability curves for a variety of geometries and operating conditions as well as demonstrate the fundamental link between heat recirculation from the post-flame to pre-flame regime and the flame speed [12].

In order to make quantitatively accurate predictions of experimental observations and to develop reliable design tools for micro-combustors, it is necessary to develop numerical models that include more accurate physical features that in analytical models are simplified. Simulations of hydrogen combustion in narrow channels have been widely conducted with detailed reaction mechanisms, exhibiting well captured combustion stabilities and flame dynamics [13-16]. However, from the practical point of view, hydrogen is a difficult fuel to use owing to its low density and safety considerations. Methane, as the largest constituent of natural gas, is a safer and more reliable candidate for small scale power generation and its mesoscale-combustion features need to be better characterised. For numerical simulations of methane/air combustion within narrow channels, most works have been carried out for steady-state models and there is limited publication involving detailed reaction chemistry. Lee and Kwon [17] and Li et al. [18] numerically investigated the micro-flame structure and variations of flame temperature under different conditions respectively, by using the 16-species and 25-reaction skeletal mechanism of Smooke and Giovangigli [19], however, this reaction chemistry was reported to sacrifice accuracy in predicting ignition delay [20]. Gauthier et al. [21] recently used the 19-species and 84-reaction methane/air chemistry developed by Kazakov and Frenklach (DRM19) [22] to study flame stabilization in small channels via solving two-dimensional steady-state fully elliptic equations. It was found that the DRM19 mechanism could closely reproduce the main physical features of high-temperature methane combustion. More importantly, as the subset of a full GRI-Mech3.0 chemistry (an optimized chemical kinetics designed to model natural gas combustion), this truncated mechanism DRM19 was able to save computational cost but was also proved to provide accurate modelling of ignition delay and heat release [20] and therefore is applicable for transient numerical simulations.

The objective of the present work is to increase the understanding of methane-air flame stability in channels using a high fidelity chemical reaction scheme along with 2-D effects. This is done via time accurate numerical simulations of flames of pre-heated methane-air mixtures in a narrow, heated parallel channel using the detailed chemical kinetics model (DRM19) to provide insight into the gas-phase homogeneous reactions and thermal trade-offs.

Numerical Approach

The flame propagation and flame dynamics in a two-dimensional, planar micro-channel are numerically studied by using the Eilmer code [23], which is an in-house Navier–Stokes solver for transient, compressible flow in 2/3-D developed at the University of Queensland. The cell-centred, finite volume method is employed for the discretization of the governing equations. Time-accurate and numerically stable solutions are obtained by setting the Courant-Friedrichs-Lewy (CFL) value to 0.3 to choose the simulation time step and using the explicit three-stage Runge-Kutta time-stepping scheme.

Figure 1 shows the computational domain/grids and boundary conditions used for the numerical model. The combustor length is 5 mm and channel height is 600 microns. A plenum upstream of the combustor with the length of 3 mm and the maximum height of 5 mm is also simulated to minimize the effect of the inlet boundary. The boundary conditions are as follows. The plenum inlet is set as subsonic boundary condition in which the total pressure (P_0) and temperature (T_0) are set. The combustor exit is set at atmospheric pressure. At the wall of the plenum, a fixed temperature ($T_{plenum} = T_0$), no-slip boundary condition is applied. At the wall of the combustor, a hyperbolic tangent temperature profile (as done in [15,16]) is employed: it ramps from T_0 to a high temperature T_w over the initial 1 mm of the whole combustor length while maintains at T_w for the remaining 4 mm of the combustor. Due to the assumption of symmetry for the

small channel, only half of the channel is simulated such that no diffusion and convective flux is applied across the centreline.

A total of 420 × 16 cells are uniformly distributed in the stream-wise and span-wise direction over the combustor while for the plenum a total of 100 × 16 cells with a built-in clustering scheme is used to mesh the grid finer near the junction to the combustor and coarser elsewhere to save computational cost. Grid refinement study was performed by comparing the methyl (CH_3) radical concentration profile along the centreline for several gird sizes (not shown here). The grid resolution used here was found to be adequate for spatial accuracy as the CH_3 concentration peak and its position were not significantly affected when finer resolution was adopted.

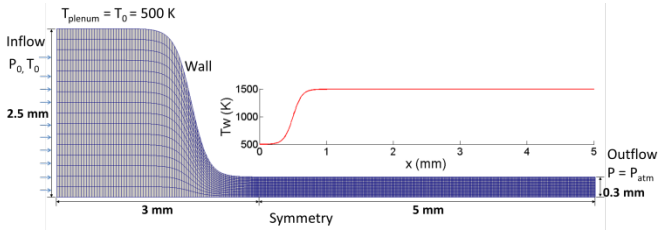

Figure 1. Computational domain of the planar half channel and boundary conditions used.

As mentioned above, the DRM19 methane/air reaction mechanism is used in the model to capture the ignition delay and flame behaviours. The simulations were performed in parallel with each simulation using 64 computational nodes and taking 60 - 100 hours of wall clock time on the national research computing cluster Raijin [24] for a typical simulation time of 7 - 10 ms.

Results and Discussion

In order to quantitatively characterize the process of combustion ignition and flame propagation, the chemical heat release rate (HRR) is calculated according to the definition:

$$HRR = \sum \dot{\omega}_s h_s \qquad (1)$$

where $\dot{\omega}_s$ is the summation of production/loss rates of species s over all reactions and h_s is the standard enthalpy of formation of species s.

By integrating HRR over the whole computational domain, the total heat release rate (THRR) is represented as

$$THRR = \int_V \sum \dot{\omega}_s h_s dV \qquad (2)$$

For all simulations, preheated CH_4/Air mixture at the pressure differential $\Delta P = (P_0 - P_{exit})/P_{exit} = 5 \times 10^{-5}$, total temperature T_0 = 500 K, equivalence ratio $\Phi = 1.0$ is supplied at the inlet. Two maximum combustor wall temperatures T_w (1500 and 1400 K) are simulated to study the effect of the wall temperature on the flame propagation inside the channel.

Spatially stable flame (T_w = 1500 K)

Figure 2 plots the temporal evolution of the flame for the case of T_w = 1500 K in the combustor section. As the premixed CH_4/air mixture flows through the channel, it gets heated by the "hot" walls. After an initial time delay (ignition delay), methyl (CH_3) radicals are formed at the channel exit. At around 2 ms, the flame is initialized and starts to propagate upstream within the channel at a quite high flame speed (up to several metres per second). Apart from methyl radicals and some carbon species e.g. formaldehyde (CH_2O) which are responsible for the establishment of the flame front, other radicals/intermediates such as carbon monoxide (CO), hydroxyl (OH) and hydrogen atom (H) and products such as water (H_2O) and carbon dioxide (CO_2) are produced via subsequent reactions downstream of the primary combustion front.

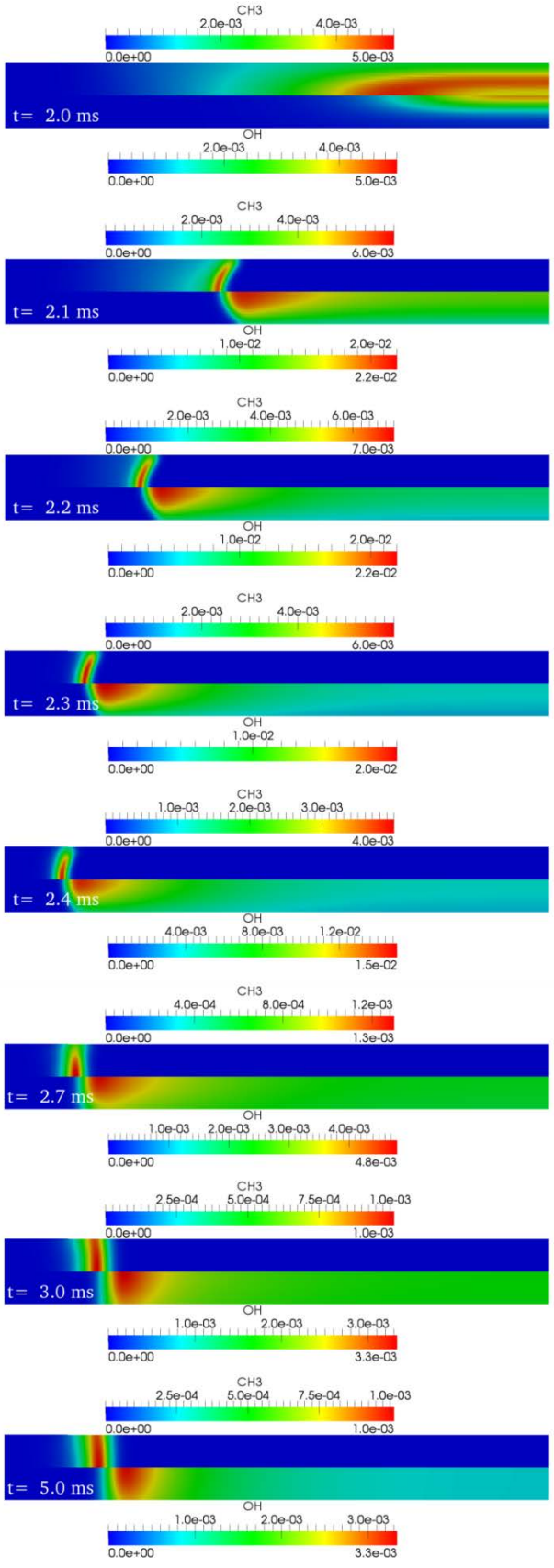

Figure 2. Temporal evolution contours of CH_3 and OH mole fractions (upper and lower half channel respectively) for T_0 = 500 K, $\Delta P = 5 \times 10^{-5}$, $\Phi = 1.0$, $T_w = 1500$ K.

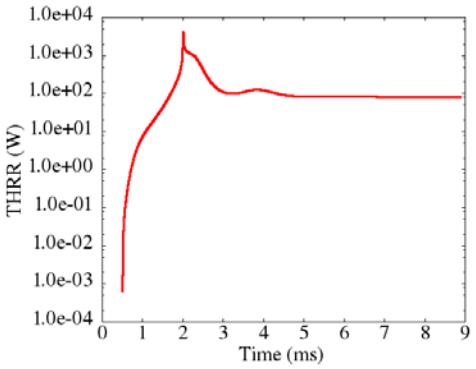

Figure 3. Total heat release rate throughout simulation time for T_0 = 500 K, P_0 = 1.00005 atm, Φ = 1.0, T_w = 1500 K.

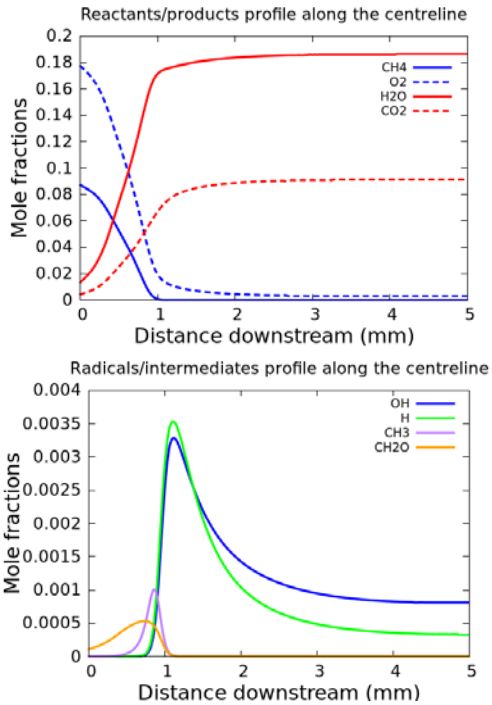

Figure 4. Species mole fraction profiles along the centreline for T_0 = 500 K, P_0 = 1.00005 atm, Φ = 1.0, T_w = 1500 K, at t = 5.0 ms.

The temporal evolution of the total heat release rate throughout the whole simulation time is shown in Figure 3. Since the reaction time scale is much shorter than the transverse heat conduction time scale, the chemical heat release rate peaks at a fairly high value (~4000 W) within a quite short time after ignition. As the flame propagates within the channel, the flame speed starts decreasing and the THRR also decreases due to the decreased gas temperature owing to heat losses from the flame zone to the wall. The flame speed gets balanced with the mixture mean flow velocity and the flame tends to be stabilized after 3 ms. The flame finally evolves to a quasi-steady state after 5 ms with the THRR reaching a relatively stable value (~80 W). The mole fraction profiles of combustion reactants/products and some radicals/intermediates along the channel centreline for the stable flame are plotted in Figure 4.

Flame with repetitive extinction and ignition (T_w = 1400 K)

At a lower wall temperature of 1400 K, longer ignition delay (~ 5.7 ms) is observed due to the slower heating rate by the wall. On the other hand, after the reaction is triggered, larger transverse temperature gradient at a lower wall temperature leads to larger heat losses from the flame to the wall, which is unfavourable for sustaining a stable combustion. As a result, an interesting flame dynamics i.e. flame with repetitive extinction and ignition (FREI) is induced (Figure 5): Flame after ignition at exit of the channel travels upstream rapidly accompanied by large heat losses which weakens the flame during the propagation process. The flame cannot be sustained and eventually extinguishes when reaching the cold inflow. Subsequently, the unburnt gas mixture refills in the channel and is heated up by the wall, which marks the prelude to the next cycle. The temporal evolution of the total heat release rate within the combustor (Figure 6) successfully captures this interesting micro-flame behaviour. By taking a fast Fourier transform (FFT), the predominant frequency of the FREI is determined to be ~100 Hz (Figure 7).

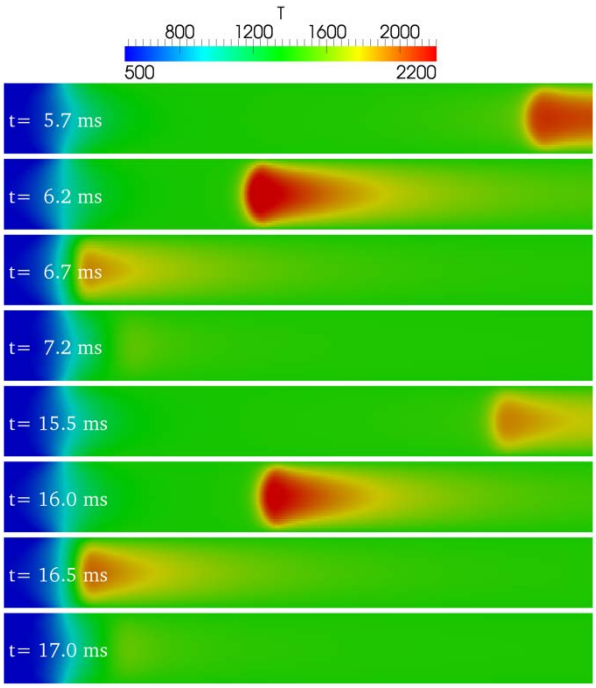

Figure 5. Temporal evolution contours of temperature showing repetitive extinction and ignition for a lower T_w = 1400 K.

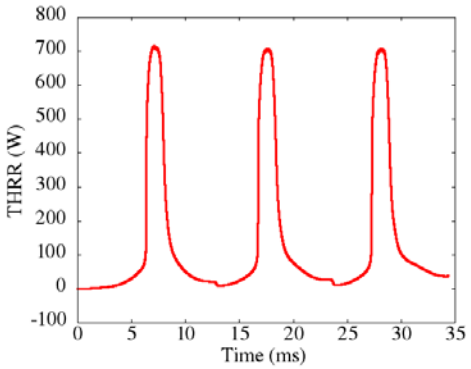

Figure 6. Temporal evolution of total heat release rate for T_w = 1400 K.

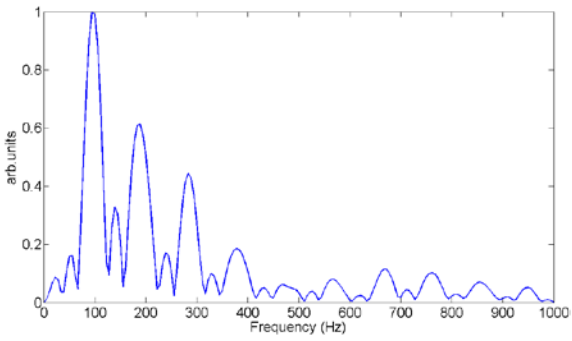

Figure 7. Fast Fourier transform (FFT) of the total heat release rate.

Conclusions

Simulations of premixed methane/air combustion with detailed chemistry were performed for flame propagation in narrow, heated channels. The effects of the combustor wall temperature on the flame behaviours were investigated by monitoring the variation of the total heat release rate within the channel. For the wall maximum temperature of 1500 K and 1400 K, spatially stable flames and flames with repetitive extinction and ignition (FREI) were observed respectively. The effects of other parameters such as mixture equivalence ratio, channel height and length on the flame propagation will be examined in future work.

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References

[1] Leach, T.T., Cadou, C.P., The Role of Structural Heat Exchange and Heat Loss in the Design of Efficient Silicon Micro-combustors, *P COMBUST INST.*,**30**, 2005, 2437-2444.

[2] Ju, J., Maruta, K., Microscale Combustion: Technology Development and Fundamental Research, *Prog Energ Combust.*,**37**, 2011, 669-715.

[3] Kaisare, N.S., Vlachos, D.G., A Review On Microcombustion: Fundamentals, Devices and Applications, *Prog Energ Combust.*,**38**, 2012, 321-359.

[4] Kim, N.I., Kato, S., Kataoka, T., Yokomori, T., Maruyama, S., Fujimori, T., Maruta, K., Flame Stabilization and Emission of Small Swiss-roll Combustors as Heaters, *COMBUST FLAME.*,**141**, 2005, 229-240.

[5] Evans, C.J., Kyritsis, D.C., Operational Regimes of Rich Methane and Propane/Oxygen Flames in Mesoscale Non-adiabatic Ducts, *P COMBUST INST.*,**32**, 2009, 3107-3114.

[6] Heatwole, S., Veeraragavan, A., Cadou, C.P., Buckley, S.G., In Situ Species and Temperature Measurements in a Millimeter-Scale Combustor, *NANOSC MICROSC THERM.*,**13**, 2009, 54-76.

[7] Maruta, K., Kataoka, T., Kim, N.I., Minaev, S., Fursenko, R., Characteristics of Combustion in a Narrow Channel with a Temperature Gradient, *P COMBUST INST.*,**30**, 2005, 2429-2436.

[8] Fan, A., Minaev, S., Kumar, S., Liu, W., Maruta, K., Regime Diagrams and Characteristics of Flame Patterns in Radial Microchannels with Temperature Gradients, *COMBUST FLAME.*,**153**, 2008, 479-489.

[9] Ronney, P.D., Analysis of Non-adiabatic Heat-recirculating Combustors, *COMBUST FLAME.*,**135**, 2003, 421-439.

[10] Leach, T.T., Cadou, C.P., Jackson, G.S., Effect of Structural Conduction and Heat Loss on Combustion in Micro-channels, *COMBUST THEOR MODEL.*,**10**, 2006, 85-103.

[11] Ju, Y., Xu, B., Theoretical and Experimental Studies on Mesoscale Flame Propagation and Extinction, *P COMBUST INST.*,**30**, 2005, 2445-2453.

[12] Veeraragavan, A., Cadou, C.P., Flame Speed Predictions in Planar Micro/Mesoscale Combustors with Conjugate Heat Transfer, *COMBUST FLAME.*,**158**, 2011, 2178-2187.

[13] Kim, N.I., Maruta, K., A Numerical Study on Propagation of Premixed Flames in Small Tubes, *COMBUST FLAME.*,**146**, 2006, 283-301.

[14] Li, J., Chou, S.K., Li, Z.W., Yang, W.M., A Comparative Study of H_2-air Premixed Flame in Micro Combustors with Different Physical and Boundary Conditions, *COMBUST THEOR MODEL.*,**12**, 2008, 325-347.

[15] Pizza, G., Frouzakis, C.E., Mantzaras, J., Tomboulides, A.G., Boulouchos, K., Dynamics of Premixed Hydrogen/Air Flames in Microchannels, *COMBUST FLAME.*,**152**, 2008, 433-450.

[16] Pizza, G., Frouzakis, C.E., Mantzaras, J., Tomboulides, A.G., Boulouchos, K., Dynamics of Premixed Hydrogen/Air Flames in Mesoscale Channels, *COMBUST FLAME.*,**155**, 2008, 2-20.

[17] Lee, K.H., Kwon, O.C., A Numerical Study on Structure of Premixed Methane–air Microflames for Micropower Generation, *CHEM ENG SCI.*,**62**, 2007, 3710-3719.

[18] Li, J., Chou, S.K., Yang, W.M., Li, Z.W., A Numerical Study on Premixed Micro-combustion of CH_4–air Mixture: Effects of Combustor Size, Geometry and Boundary Conditions on Flame Temperature, *CHEM ENG J.*,**150**, 2009, 213-222.

[19] Smoke, M., Giovangigli, V., *Reduced Kinetic Mechanisms and Asymptotic Approximations for Methane-Air Flames*, Springer Berlin Heidelberg, 1991.

[20] O'Flaherty, B., *Reducing the Global Warming Potential of Coal Mine Ventilation Air by Combustion in a Free-piston Engine*, PhD Thesis, The University of Queensland, Australia, 2012.

[21] Gauthier, G.P., Watson, G.M.G., Bergthorson, J.M., An Evaluation of Numerical Models for Temperature-Stabilized CH4/Air Flames in a Small Channel, *COMBUST SCI TECHNOL.*,**184**, 2012, 850-868.

[22] Kazakov, A., Frenklach, M., *Reaction Set DRM19*, http://www.me.berkeley.edu/drm/, accessed June 2014.

[23] Gollan, R.J., Jacobs, P.A., About the Formulation, Verification and Validation of the Hypersonic Flow Solver Eilmer, *INT J NUMER METH FL.*,**73**, 2013, 19-57.

[24] National Computational Infrastructure Raijin system, http://nci.org.au/nci-systems/national-facility/, accessed June 2014.