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On the effect of outflow boundary truncation for numerical simulation of narrow-channel flames

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Abstract

Premixed methane/air flame propagation in a two-dimensional, planar micro-channel is modelled by solving the transient, full Navier–Stokes equations with the reaction mechanism DRM-19 using our in-house code (Eilmer). Effects of two different outflow boundary treatments, i.e. applying an outflow boundary truncation and using a domain-extension joining the combustor outlet are investigated, for both steady-state flames and periodically oscillating flames. It is found that the use of a domain truncation/extension mainly influences the acoustic wave damping time at the initial stage when the flame is initiated. For the steady-state flame case, there is no noticeable difference in final solutions between two outflow treatments. For the spatially oscillating flames, the characteristics in terms of the oscillation frequency and amplitude are slightly but not significantly affected when the flame settles into a consistent oscillatory pattern.

Introduction

Micro/mesoscale combustion, which can be viewed as combustion in narrow passages typically on the order of flame thickness, finds application in portable power systems and small scale propulsion systems [3, 5]. In order to provide design/operation guidelines for such small-scale systems, it is important to make quantitatively accurate predictions of flame behaviours. Due to the difficulties of experimentally conducting spatially resolved measurements owing to the small size of these systems, numerical simulation becomes an important tool to reveal spatially and temporally resolved flame features.

Simulations of micro/mesoscale combustion for a variety of fuel/oxidiser systems, using global/detailed reaction mechanisms, have been widely performed in literature, exhibiting combustion stabilities and various flame dynamics [1, 14, 9, 4]. These studies, typically simulated a subsonic combustor domain in a relatively simple geometry (cylindrical or planar channel) with an outlet that was "truncated" from the rest of the lab. This involved applying an outlet boundary condition of constant ambient pressure directly at this truncated boundary. However, there is limited literature discussing the appropriateness of adopting this convention. Some influence of that truncation on the channel flow might be expected, in particular on the acoustic waves pattern due to this approximation. In order to investigate this, in this paper the flame propagation in a parallel-plate micro-channel is simulated, with the same outflow boundary truncation as done in these other works in literature, as well as boundary condition applying a domain-extension joining the combustor to capture the "realistic" presence of the quiescent ambient in the real world.

Numerical Approach

Premixed CH_4/air combustion in a planar two-dimensional narrow channel is simulated using our in-house code Eilmer [2] for transient, compressible flows. A cell-centred, finite volume method is employed for the discretisation of the governing compressible Navier–Stokes equations. An explicit, three-stage *Runge-Kutta* scheme is used for the time-marching. Within a single time-step, the physical processes of fluid dynamics (inviscid and viscous fluxes) and chemistry (combustion reactions) are updated sequentially in a decoupled fashion, using the operator-splitting method. In order to obtain time-accurate and numerically stable solutions, the *Courant-Friedrichs-Lewy* (CFL) number is set to 0.45 to choose the simulation time step (on the order of 10^{-9} s). The details of these solver numerics can be found in [2].

The evaluation of thermodynamic and transport properties for the component species used curve fits collated by McBride and Gordon [7] 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 [15] for transport properties. Fick's law, using mixture-averaged diffusion coefficients [10], was implemented to evaluate the species mass diffusion. A correction for calculated fluxes was performed in order to guarantee total mass conservation numerically [13]. The simulations used the 19-species and 84-reaction methane/air chemical kinetics (DRM-19) [6]. As the subset of a full GRI-Mech chemistry [12], this truncated mechanism DRM-19 is able to save computational costs and has also been proved to provide accurate modelling of heat release and ignition delay [8], as well as laminar burning velocity [11] against experimental data, and can therefore be considered to closely reproduce the main physical features of transient flames. Validation work of the model for simulating a premixed methane/air combustion in a small channel was reported in our previous article [4], showing that this mechanism captured the flame structure well.

Figure 1 shows the computational domain in this paper. The combustor is a parallel-plate micro-channel (bounded by the red dashed-lines in the figure), with the dimensions of 6 mm $\times$ 0.6 mm in length (L) and height (H) respectively. The boundary conditions were set as follows: 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 of the stoichiometric mixture, and a uniform mass flux ($\dot{m}''$) across the boundary were specified. At the walls of the combustor, a no-slip boundary condition with a prescribed hyperbolic tangent temperature profile to mimic the heat recirculation via wall conduction (as done in [9, 4]) was employed. The temperature ramps from the mixture inlet temperature of 300 K to a high temperature at 1400 K, with the largest temperature gradient of 2200 K/mm at the middle of the channel length (shown in Figure 1).

As mentioned earlier, two types of outflow boundary treatments were used. For applying the outflow boundary truncation, the pressure was set at atmospheric pressure at the combustor outlet, while zero *Neumann* boundary conditions were imposed for the rest of the variables. For the case of the domain-extension joining the combustor outlet, the outlet boundary was moved to the right end of the extended domain, with the same settings

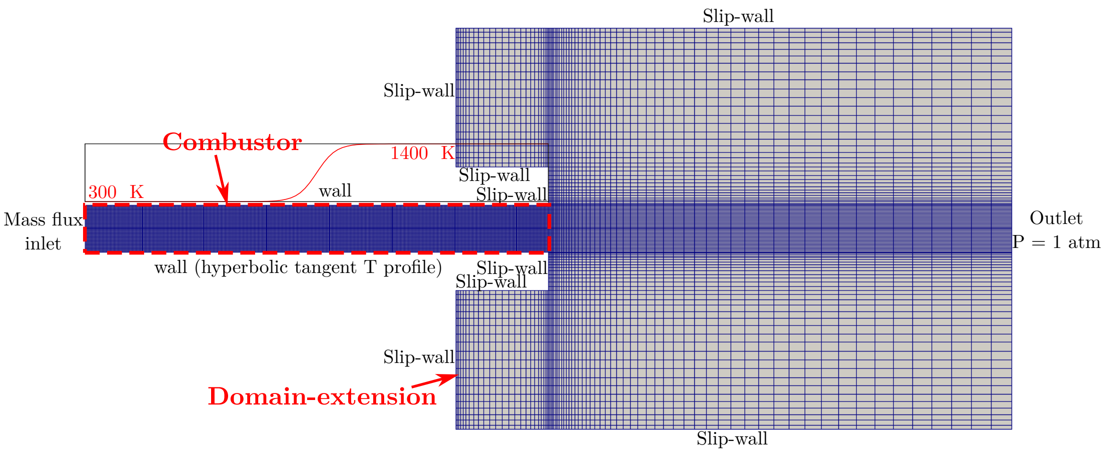

Figure 1: Computational domain showing the truncated planar combustor and the domain-extension joining the combustor outlet.

applied (atmospheric pressure + zero *Neumann* for other variables). The extended domain is a buffer zone with back steps (see Figure 1), within which the acoustic waves generated due to gas density changes during combustion are expected to be damped out. A simple slip wall condition (simulating a solid wall with no viscous effects) was used for the rest of boundaries of the domain-extension.

A uniform mesh consisting of 354×36 cells with the cell size of 17.0 μm was employed in the combustor (red dotted zone shown in Fig. 1) to preserve the same spatial accuracy throughout the domain. A grid refinement study was performed for a steady-state flame case by comparing the temperature and species concentration profiles along the channel centreline for several mesh levels (not shown here). This refinement study identified the mesh resolution chosen above as being sufficient as the flame was invariant to further grid refinement. For the domain-extension, the mesh density in the connection region is comparable to that within the combustor zone to ensure a smooth transition, while is much coarser elsewhere to save computational cost.

An "ignition-zone" was used to initiate the flame. An artificial rate-controlling temperature (set at 1800 K) was used in the "ignition-zone" (located between $0.75L$ - $0.8L$) to inflate the Arrhenius chemical reaction rate while keeping the thermodynamic temperature as per the flow condition. This zone was in effect for the first 0.5 ms of the simulation time to ignite the flame and then "switched-off" subsequently. The "ignition-zone" method merely saves some computational cost, as compared to the case where the flame "auto-ignites" due to the hot wall, while does not influence the solutions after the flame is initiated.

Results and Discussions

Combustion of stoichiometric mixture at two inflow velocities U_{in} 0.4 and 0.2 m/s (equal to the laminar flame speed and half of the laminar flame speed) was studied. Two flame behaviours namely steady-state flames and periodically oscillating flames were observed at the two inlet velocities respectively. In the following discussions, an important quantity of the *total heat release rate* (*THRR*) over the combustor zone is used to characterise the flame. It is computed as:

$$THRR = -\int_V \sum_{s=\text{all}} \dot{\omega}_s h_s \, dV, \qquad (1)$$

where $\dot{\omega}_s$ and h_s are the production/loss rate and the standard enthalpy of formation of species s respectively. During simulations, a point located at the centre of the combustor zone is monitored for the temporal variation of the pressure.

Steady-state Flames (U_{in} = 0.4 m/s)

At the inflow velocity equal to the laminar flame speed (0.4 m/s for CH_4-Air flames), flames for both types of outflow boundary treatments have steady solutions, representing flame stabilisation. At the start of the simulation when the flame is initiated, owing to the drastic change in the flow temperature and density, a considerable amount of acoustic waves are generated that propagate back and forth within the channel, leading to large pressure oscillations. Within a certain period of time, these oscillations are gradually damped out. However, as shown in Figure 2, this wave-damping time for the domain-truncation case is shorter than that for the domain-extension case, mainly owing to the shorter wave-propagation distances. After the "ignition event", the flame gradually propagates upstream and eventually evolves to its steady state.

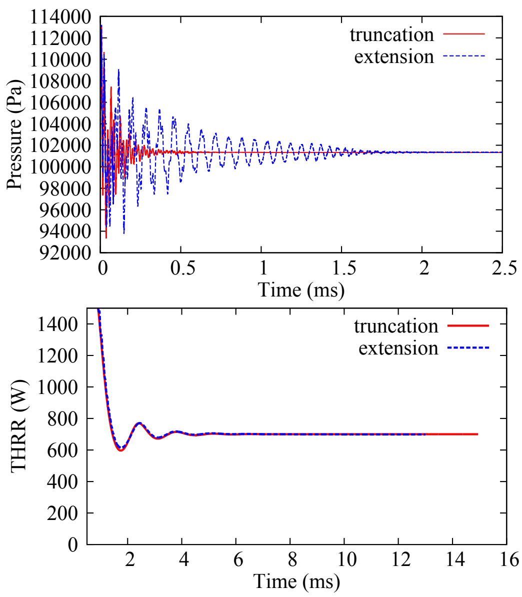

Figure 2: Pressure variations at the monitored point (located at the centre of the combustor zone) and *THRR* evolutions for two types of outflow boundary treatments, at U_{in} = 0.4 m/s.

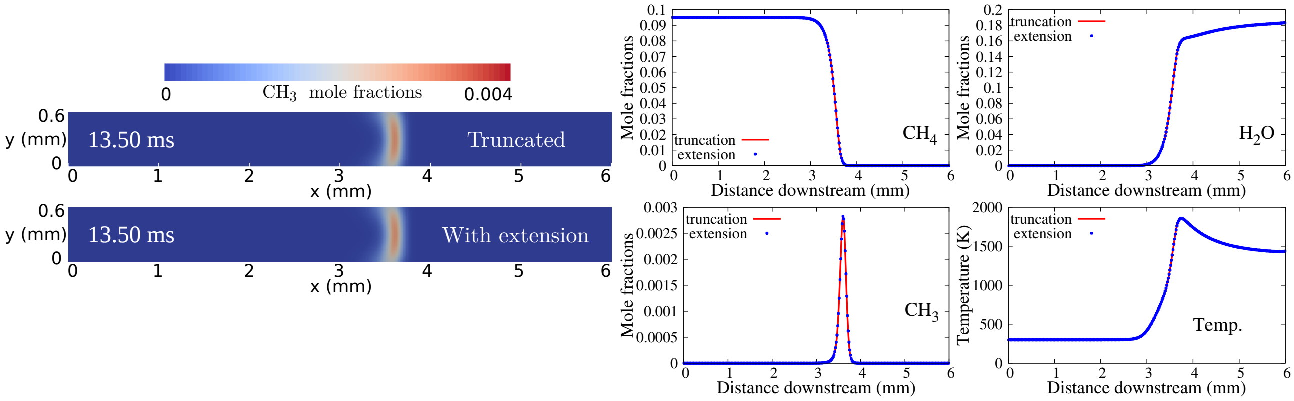

Figure 3: Contour of CH_3 mole fractions (left), and profiles of species and temperature along the channel centreline (right) of the steady-state flame solutions (U_{in} = 0.4 m/s), using a truncated computational domain and a domain with an extension.

This can be reflected by the *THRR* variation in Figure 2: The *THRR*s time evolution behaviour is similar for both cases, and asymptotically approaches a steady-state values of ∼700 W. Figure 3 shows the contour of methyl radical (CH_3) mole fractions and sliced profiles of species and temperature along the channel centreline for the flame at its steady state (t = 13.5 ms). CH_3 mole fraction is used to represent the flame front [4]. It is found that the flames are stabilised at the same location along the channel streamwise direction between two outflow boundary treatments. There is no noticeable difference in both the CH_3 mole fraction contours, and the sliced profiles of species and temperature. Therefore, it is believed that the outflow boundary truncation does not influence the steady-state flame solutions.

Oscillating Flames (U_{in} = 0.2 m/s)

At U_{in} equal to half of the laminar flame speed of 0.2 m/s, the wave-damping behaviours at the flame initiation stage are found to be quite similar to those at U_{in} = 0.4 m/s. As shown in Figure 4, the domain-extension case is still characterised with longer wave-damping time compared to the domain-truncation one. However, unlike the simulations at U_{in} = 0.4 m/s showing flame stabilisation, flames are found to exhibit spatial oscillations at the lower inflow velocity. The oscillation amplitudes, first increase with time gradually, and then maintain at a stable periodic level after t = ∼20 ms. However, the differences between the truncation and domain-extension cases are still small. As discussed in our previous work [4], this flame spatial oscillation, can be viewed as a competition between the flame propagation speed and the local flow velocity. The flame propagation speed, is weakened in the flame-upstream-moving phase due to the large surface heat losses, while is enhanced during the flame-downstream-moving phase owing to the increased wall-preheating length.

Figure 5 shows the flame temporal evolutions within one oscillation cycle, for the simulations using a truncated computational domain and the domain with an extension. The case using the domain-extension is found to have a slightly larger flame spatial oscillation, compared to its domain-truncation counterpart (from 3.28-4.14 mm vs from 3.28-4.08 mm along the channel length). By taking a *fast Fourier transform* (FFT) of the temporal evolution of the *THRR*, the predominant frequencies of the oscillating flames are determined. Calculated values for the domain-truncation and domain-extension case are close to each other (430.5 Hz vs 424.9 Hz), as shown in Figure 6.

Therefore, the use of outflow boundary truncation is believed to exert a limited effect for the spatially oscillating flames, only

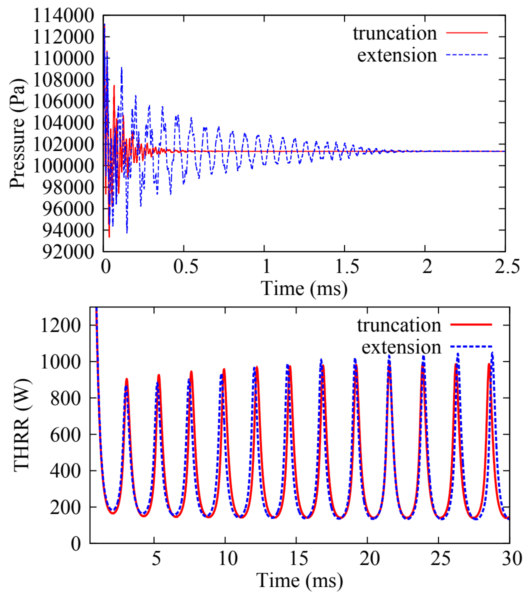

Figure 4: Pressure variations at the monitored point (located at the centre of the combustor zone) and *THRR* evolutions for two types of outflow boundary treatments, at U_{in} = 0.2 m/s.

leading to a small difference in both the oscillation amplitude and frequency, compared to the domain-extension treatment.

Conclusions

This paper investigated the effect of different outflow boundary treatments for numerical simulation of narrow-channel flames, using the transient, compressible flow solver Eilmer. Simulation results for applying the outflow boundary truncation and using a domain-extension joining the combustor outlet were compared. The use of the domain truncation/extension was found to mainly influence the wave-damping characteristics at the flame initiation stages. For the stabilised flames, there was no noticeable difference in the steady-state solutions between two outflow treatments. For the periodically oscillating flames, the oscillation frequency and amplitude were only slightly affected. Therefore, the outflow boundary truncation can be regarded as a reasonable simplification for simulating a micro-flame propagation problem.

Acknowledgements

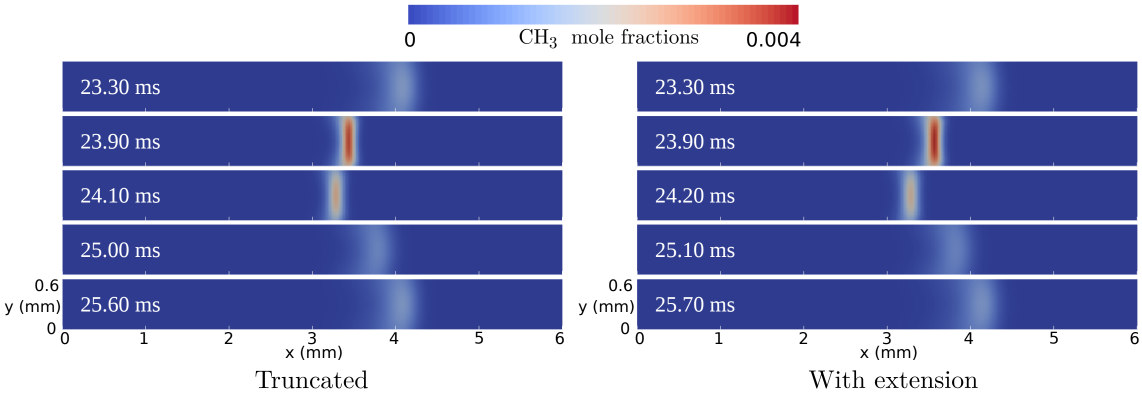

Figure 5: Temporal evolution of the oscillating flames (U_{in} = 0.2 m/s) within one cycle, using a truncated computational domain and a domain with an extension.

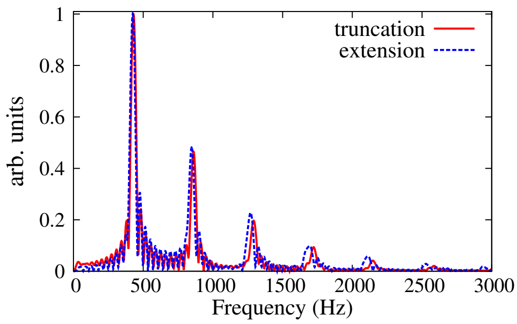

Figure 6: *Fast Fourier transform* of the *THRR* for two types of outflow boundary treatments, showing the predominant frequencies of flame oscillations.

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