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Two-dimensional simulation of premixed laminar flame at microscale

Zerrin Turkeli-Ramadan *, Rajnish N. Sharma, Robert R. Raine

Department of Mechanical Engineering, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

HIGHLIGHTS

- 2D numerical simulation of premixed methane–air flame at small scale was performed.
- Preheating the reactants widens the flame stability at high incoming flow velocity.
- Correa's mechanism was applied to premixed laminar methane–air flame successfully.
- Applying low target residual for convergence is important to obtain an accurate solution.

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ABSTRACT

Microcombustion is one of the most essential topics in the development of micropower generators for portable devices, microaerial vehicles and sensors. Although one-dimensional numerical modelling of combustion has been developed, maturing a lot during the last forty years, two-dimensional numerical modelling of combustion, particularly at very small scales has only started in the last decade. In this particular study, two-dimensional numerical simulations of premixed, laminar, lean methane–air flames at atmospheric pressure formed in a 2 mm diameter microcombustor are performed. A skeletal mechanism consisting of 16 species and 41 reactions is employed. This study shows the importance of applying low target residuals for convergence in CFD, which plays a critical role in obtaining an accurate solution in the numerical modelling of microcombustion. The main focus of this work is to investigate the effect of preheating the reactants on the flame structure and stability with adiabatic and non-adiabatic combustor walls. The flame in the 2 mm diameter circular microcombustor under adiabatic wall conditions shows a laminar Bunsen type flame behaviour. On the other hand, under the non-adiabatic wall conditions, a cone shaped high temperature flame zone is observed. Preheating the reactants widens the flame stability at high incoming flow velocities under both conditions, however, under non-adiabatic wall conditions, at low incoming flow velocities and/or low mass flow rates, preheating the reactants contributes neither to flame stability nor combustion characteristics. On the contrary, it results in low combustor exit temperature. Finally, the effects of convective heat transfer coefficients and heat loss, with and without radiation, on the microcombustion are analysed.

1. Introduction

Microcombustors are the main components of microheat engines, microgas turbines, and micro-thermoelectric and thermo-photovoltaic systems. The development of these systems has been accelerated recently with the increasing necessity of efficient power sources for portable electronics and miniature mechanical devices. These proposed power supplies have the potential to provide increased lifetime and reduced weight compared to batteries. In comparison, combustion of hydrocarbon and hydrogen fuels offers much higher power and energy density than batteries. This makes harnessing of energy from microcombustion an attractive alternative pathway to the realisation of the miniaturisation of power sources (Chou et al., 2011; Fernandez-Pello, 2002; Ju and Maruta, 2011; Maruta, 2011).

Downscaling the combustor into millimetric size introduces new problems that do not occur in conventional combustors, such as shorter residence time, and relatively higher heat losses. These result in flame quenching, incomplete combustion and increased pollutant emissions (Guidez et al., 2005; Sakurai et al., 2009; Waitz et al., 1998; Yuasa et al., 2005).

Generally in microcombustors, the flame stability limit has a U shape in terms of mass flow rate (or incoming flow velocity) versus equivalence ratio (Yuasa et al., 2007). As the size of the

* Corresponding author. Tel.: +64 9 923 8144; fax: +64 9 373 7479.
E-mail address: ztur002@aucklanduni.ac.nz (Z. Turkeli-Ramadan).

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combustor decreases, the surface area-to-volume ratio increases. Heat loss is proportional to the surface area while heat release is proportional to the volume. As the surface area-to-volume ratio increases, the ratio of heat loss to heat release also increases. At low mass flow rates, heat loss is higher than the heat release rate causing flame extinction. On the other hand, at high mass flow rates, the incoming flow velocity becomes higher than the burning velocity, which in turn results in blow out.

Widening the flame stability limit can be achieved by increasing the reactant temperature (Lee et al., 2008; Turkeli-Ramadan et al., 2011). As the size of the combustor decreases, the residence time gets shorter. In order to obtain complete combustion, the residence time should be longer than the chemical reaction time. Increasing the reactant temperature shortens the chemical reaction time thus assuring completion of the combustion process within microcombustors.

It is also well known that preheating the reactant increases the burning velocity. Andrews and Bradley (1972) showed the dependence of burning velocity (S) on reactants temperature (T_u) empirically for methane–air flames at atmospheric pressure. They obtained the following formula for the laminar burning velocity of stoichiometric methane–air flames

$$S = 10 + 0.0003717T_u^2\ (\mathrm{cm/s}),\ \ 150\ \mathrm{K} < T_u < 1000\ \mathrm{K} \tag{1}$$

Particularly at higher mass flow rates (or higher incoming flow velocities), increasing the reactant temperature raises the burning velocity and prevents blow out, thus widening the flame stability limit. Lee et al. (2008) showed experimentally the effect of increasing the reactant temperature up to 500 K on the flame stability of microflames on a microtube. Turkeli-Ramadan et al. (2013) have also presented experimental data showing the widening of the flame stability limit by preheating the reactant temperature up to 600 K with a somewhat larger size combustor. Li et al. (2009a) numerically investigated the effect of elevated temperatures up to 500 K on the stability of flames from hydrogen–air, methane–air and propane–air mixtures with a 1D model. It was found that when the reactant temperature increases, the heat loss ratio (defined as the ratio of heat loss from the flame to the heat generation in the reaction zone) drops substantially for these three different fuel–air mixtures. However they neither reported on the species concentrations nor studied the effects of incoming flow velocity. The study focused mainly on heat loss ratio and heat recirculation ratio.

The difficulty of performing experiments at very small scales makes numerical simulation an essential part of microcombustion research. The numerical approach has been widely employed, particularly in microcombustors whose size is less than the quenching distance, which is a few millimetres for hydrocarbon fuels and even smaller for hydrogen.

One-dimensional premixed methane–air flames have been widely investigated numerically since the beginning of the 1980s. However, when combustor size is of significance, two-dimensional modelling of microcombustion has gained importance. Research on the two-dimensional numerical simulation of microcombustion has emerged with the increasing interest in combustion-based micropower generators. Due to its less complex reaction mechanisms when compared to hydrocarbon reaction mechanisms, pioneering two-dimensional microcombustion studies were performed on hydrogen microcombustion (Hua et al., 2005a, b; Verstraete et al., 2005). There are very few studies performed with two-dimensional numerical modelling of premixed methane–air flames at microscale (Li et al., 2009c; Norton and Vlachos, 2003).

1D simulations of methane–air flame have been widely investigated and validated with experimental data. However, 2D simulations, especially at microscale, are a new developing area. 2D simulations at microscale found in the literature used the commercial Computational Fluid Dynamics (CFD) software package ANSYS Fluent (2010). Since it is a new area and has been investigated only in the last decade, this paper next looks at previous studies on microcombustion in 2D using ANSYS Fluent, and their shortcomings.

Verstraete et al. (2005) and Hua et al. (2005a, b) investigated hydrogen combustion in both a microtube combustor and the geometry of MIT's ultra micro gas turbine (UMGT). However, hydrogen is not a good candidate for small portable devices because of its storage problems, although its high heating value, and high burning velocity are advantages over other hydrocarbons (Decuypere and Verstraete, 2005). Therefore, methane is chosen as a fuel, due to the fact that methane has an energy density almost 60 times higher than that of currently available lithium ion batteries (Ju and Maruta, 2011).

Lee and Kwon (2007) investigated methane–air microflames on microtubes of different sizes. Although they investigated the effect of increasing the initial temperature on the flame stability, the results of premixed jet flames were found to exhibit different characteristics to premixed flames inside the microtube.

Norton and Vlachos (2003, 2004) performed a 2D numerical study of both methane–air and propane–air mixtures with a global one-step reaction mechanism. It was found that the microcombustor dimensions strongly affect thermal stability and wall thermal conductivity is vital in determining the flame stability. Li et al. (2009c) investigated the effects of the microcombustor size and geometry, inlet velocity profile, and the slip-wall boundary condition on methane–air flame temperatures. In these studies, the predictions of flame temperature and stability mechanisms at microscale were investigated, with either a one-step reaction mechanism (Norton and Vlachos, 2003, 2004) or a skeletal mechanism with a first-order upwind scheme. But they have a major shortcoming in the use of high target residuals (1×10^{-3} for normalised RMS residuals) for convergence, particularly for the chemical species (Li et al., 2008; 2009c).

Although many pioneer analytical (Minaev et al., 2007), numerical (Kurdyumov et al., 2009; Pizza et al., 2010) and experimental (Aiwu et al., 2007; Kamada et al., 2014; Maruta et al., 2004, 2005; Sudarshan et al., 2007) studies were performed at very small scales with elevated wall temperatures or wall temperature gradients, until now no studies have been performed to investigate the effects of preheating the reactants on the flame stabilisation and the flame structure at small scales. It was found that in order to obtain a stable flame, the wall temperature should be higher than a critical value. Furthermore, these studies showed that with varying incoming flow velocities, different flame patterns (such as weak, spiral and spinning) and flame instabilities, (repetitive ignition, extinction) can be observed.

While previous studies in the area of microcombustors have focused on the effects of design factors and operating conditions, the flame structure and characteristics do not appear to have been investigated fully. These studies (Hua et al., 2005a, b; Li et al., 2008; Li et al., 2009c; Norton and Vlachos, 2003, 2004) have neither reported on major species concentrations in 2D nor on the effects of preheating on the flame characteristics. Furthermore, none of the numerical studies to date appear to have conducted a validation for their numerical model.

The main objectives of this study therefore, are to first develop a validated 2D CFD model to investigate two dimensional methane–air combustion at microscale, and to study the effects of preheating the reactants and heat loss mechanism on the flame structure and stability. A microtube combustor of a fixed size is chosen for the study.

This paper is organised as follows. Section 2 presents a brief description of the numerical model. This is followed by the simulation results and discussions in Section 3. The conclusions are summarised in Section 4.