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Numerical estimation of blowout, flashback, and flame position in MIT micro gas-turbine chamber

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HIGHLIGHTS

- Micro-combustion was simulated numerically in a 3D geometry of a micro-combustor.
- EDC combustion model is used and turbulence productions are turned off.
- Effect of omitting turbulence productions and fuel–air flow properties are studied.
- Combustor efficiency diagrams show relatively good agreement with test results.
- EDC with turbulence productions turned-off is apt for simulating micro-combustion.

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ABSTRACT

Combustion of hydrogen–air mixture has been simulated numerically inside the MIT (Massachusetts Institute of Technology) micro gas-turbine chamber. Blowout, flashback, and flame position have been studied for different equivalence ratios. Some of the considerations in this simulation are applying a 9-species, 19-step hydrogen–air reaction mechanism, thermal coupling of reacting flow and solid structure of the combustor, considering radiation and convection heat loss from the outer surface of the combustor, and exerting physical boundary conditions on 3D geometry of the combustion chamber. To solve the simulating equations for 3D computational fluid dynamics model, finite volume method has been implemented, and parallel processing has been performed on 6 compute nodes. To validate employed simulating models, the simulation results have been compared with experiment results reported from MIT laboratory and also with simulation results obtained by another research team. The comparison shows that using eddy dissipation concept model (EDC) with disabled turbulence productions and turbulent viscosity terms in k and ε transport equations and solving equations with remaining terms can predict range of mass flow for stable combustion much closer to experimental results (more than 200% improvement in simulation results), which implies that it can be considered as a relatively reliable method for modeling mean reaction rate of micro-combustion.

1. Introduction

Recently, many different kinds of micro devices such as micro-spacecrafts, air vehicles, actuators, and robots have got a lot of attention due to their various mission capabilities and also the reduction in energy consumption. Consequently, the needs for micro power-supply are increasing, especially on the power sources with high energy density (Hua et al., 2005a). On the other hand, new technology has made it possible to manufacture and assemble a new generation of micro heat engines for power generation and micro air-vehicle propulsion applications (Spadaccini et al., 2003). The combustion-based micro engines can deliver an output power density tens of times higher than the best lithium batteries ever made (Spadaccini et al., 2003). Some applications for micro-engines can be assumed as micro-propulsion, propulsion system with distributed fine thrust vectors, mobile power generator, micro-refrigerating systems, micro-controller for boundary layer and circulation, and power supply for developing micro-systems. Some of the internal combustion micro-engines and micro-power-supply concepts can be referred to as piston engine, rotary engine (Wankle), gas-turbine engine (Dumand et al., 2005), and thermo photovoltaic system (Chia and Feng, 2007).

The small dimensions of the micro-systems imply that these devices operate in a somewhat unfamiliar parameter regime (Janson et al., 1999). Recently, some experimental and numerical researches have been conducted in different aspects of micro-combustion. 2D transient simulations of methane-fueled micro-reactor with

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a platinum catalyst wall have been performed by Karagiannidis and Mantzaras (2010). These simulations were performed by varying the inlet pressure, the solid wall thermal conductivity and heat capacity, the inlet velocity, and the equivalence ratio at fuel–lean conditions. They evaluated reaction rates using CHEMKIN code. Some 3D numerical simulations of 3.5 mm wide spiral Swiss roll heat-recirculating combustors have been performed by Chen and Ronney (2011). Their simulation included finite rate chemical reaction of 1-step and 4-step propane–air mixtures, solid-phase conduction and surface-to-surface radiation. They observed that results are surprisingly similar with or without a turbulence model activated (Chen and Ronney, 2011). The combustion of H_2-air in a 2D geometry of a micro-combustor has been simulated numerically by Jejurkar and Mishra (2010, 2011a, 2011b) using the Arrhenius relation for a one-step stoichiometric hydrogen oxidation mechanism. They achieved a self-sustaining combustion under different inlet velocities and wall thermal conductivities without any need for catalyst.

Due to high power density of the micro gas-turbine which can be up to 3000 MW/m^3 (Epstein, 2003), it has been considered as one of the most-favored micro-engine concepts and one of the first power MEMS devices (Maruta, 2011; Chou et al., 2011). The power density of the MIT micro gas-turbine is approximately 1100 MW/m^3. Spadaccini et al. (2003) obtained temperature contour of the combustion chamber by employing 3D numerical simulation, and applying the chemical kinetics with a 9-species, 20-step hydrogen–air reaction mechanism. Nevertheless, the heat transfer between reacting flow and the solid combustor walls as well as the heat conduction through solid structure was not simulated in their work. Peck (2003) modeled heat transfer through solid structure of the combustor and the heat loss from this structure to the ambient, but the fluid dynamics and the combustion kinetics have not been considered in that modeling. Another numerical simulation of the MIT micro gas-turbine chamber is the work done by Hua et al. (2005b). Most of the effective parameters have been included in that simulation such as detailed chemical kinetics, fluid dynamics, heat transfer within solid structure of the combustor, and heat loss to the ambience. However, the predicted inlet mass flow rate for blowout (0.4 g/s) is far from the experiment result (0.12 g/s) reported by Mehra (2000) and also Spadaccini et al. (2003).

The 3D numerical simulation of combustion in the MIT micro gas-turbine chamber presented in this paper involves detailed chemical kinetics, thermal coupling of the reacting flow and solid structure of the combustor, and heat loss to the ambient. To model reaction rate, EDC combustion model has been employed with turbulence generations and turbulent viscosity terms eliminated from the k–ε viscous model. The effects of eliminating turbulence productions terms while using EDC model have been studied as well as the effects of inlet mass flow rate (velocity) and equivalence ratio on blowout, flashback, flame position, and burnt gas volume. Finally, combustor efficiency graphs have been plotted to be compared with experiment results reported by Mehra (2000) and Spadaccini et al. (2003) and also with simulation results achieved by Hua et al. (2005b).

2. Modeling equations and approaches

Equations and method used in this research have been described in this section as well as a concise presentation of applied chemical kinetic mechanism and numerical approach. The main assumptions of this simulation are steady-state, no gas radiations, and no surface reaction.

2.1. Modeling equations and material properties

Basic modeling equations for a reacting flow are continuity, momentum, energy conservation, species transport, and reaction rate modeling equations. Residence time for GE90 conventional combustor is about 7 ms (Spadaccini et al., 2003); while, due to the miniature volume of the micro-combustor, its residence time is approximately 0.5 ms (Spadaccini et al., 2003; Epstein, 2003). Consequently, an appropriate reaction model for micro-combustion must be sensitive to this short residence time. Regarding these conditions, EDC model has been chosen for modeling mean reaction rate, which will be discussed more in the next sections.

For all species in this simulation, density has been defined by using the ideal gas model, and specific heat capacity has been determined as a piecewise-polynomial function of temperature. Thermal conductivity, viscosity, and mass diffusivity have been modeled using the kinetic theory (FLUENT 6.3 User's Guide, 2006). Finally, the mixture physical properties have been modeled by applying the mass-weighted-mixing-law. Prior to this study, Norton and Vlachos (2003) have used the mentioned physical property models to simulate the micro scale combustion of premixed methane–air. Thermal conductivity for solid structure of silicon combustor is 149 W/m K. All mentioned modeling equations have been listed in Table 1.

2.2. Principles of EDC model

The EDC model, presents empirical expression for mean reaction rate based on assumption that chemical reaction takes place where the dissipation of turbulent energy occurs (Gran and Magnussen, 1996). These regions, according to energy cascade model, consist of fine structures with characteristic dimensions of the order of Kolmogorov micro-scale in one or two dimensions (Gran and Magnussen, 1996). At size equal to Kolmogorov micro-scale or smaller, *no turbulent structure exists* due to the fact that in those regions molecular diffusion is faster than turbulence transport (Rehm et al., 2009). Moreover, within those fine structures, reactants are mixed at a *molecular scale*, therefore, ready for chemical reactions to occur (Magnussen, 1981, 2005). The fine structure regions thus create the reaction space for non-uniformly distributed reactants (Magnussen, 2005).

EDC model assumes that the fine structures occupy only a fraction of the flow. The reactive volume fraction of the flow is ξ^3, where ξ is expressed as (Gran and Magnussen, 1996)

$$\xi = \left(\frac{3C_{D2}}{4C_{D1}^2}\right)^{1/4} \cdot \left(\frac{\nu\varepsilon}{k^2}\right)^{1/4} \tag{1}$$

Where model constants $C_{D1} = 0.134$ and $C_{D2} = 0.50$ (Gran and Magnussen, 1996) are obtained by employing energy cascade model, ν is the kinematic viscosity, and k and ε are the turbulent kinetic energy and its dissipation rate respectively. Therefore, EDC model assumes that the flow is divided into a reactive volume fraction (ξ^3), and a non-reactive part or surrounding ($1-\xi^3$). Eq. (1) implies that for low Reynolds regimes, lower turbulent kinetic energy leads to the bigger value of the ξ. The upper limit of the empirical EDC model for reactive portion of the flow is specified as 7.55E−1(Rehm et al., 2009), which has been delineated in Section 4.1.

Chemical reactions take place when reactants are *mixed at molecular scale* at sufficiently high temperature (Magnussen, 2005). The rate of *molecular mixing* is determined by the rate of mass transfer between the fine structure regions and the surrounding fluid (Magnussen, 2005). The time scale for mass transfer between fine structures and surroundings is estimated by time scale τ (Gran and Magnussen, 1996)

$$\tau = \left(\frac{C_{D2}}{3}\right)^{1/2} \cdot \left(\frac{\nu}{\varepsilon}\right)^{1/2} \tag{2}$$