

Concentration slip and its impact on heterogeneous combustion in a micro scale chemical reactor

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Abstract

The rarefied gas effect on concentration slip and on heterogeneous combustion in microscale chemical reactors was investigated. First, a concentration slip model to describe the rarefied gas effect on the species transport in microscale chemical reactors was derived from the approximate solution of the Boltzmann equation. Second, the model was verified using the direct Monte-Carlo method for the pure diffusion problems at different Knudsen numbers. The comparison showed that the present analytical model for the concentration slip boundary condition reasonably predicted the rarefied gas effect in the slip regime. Finally, the impact of the concentration slip on the coupling between the surface catalytic reactions and the homogeneous gas phase reactions in a microscale chemical reactor was examined using the one-step overall surface reaction model with a wide range of Knudsen and Damköhler numbers. It was shown that the rarefied gas effect significantly reduced the reaction rate of the surface catalytic oxidization for large Knudsen numbers. Furthermore, it was shown that the impact of slip effects on catalytic reactions strongly depends on the competition between the reaction rate and diffusion transport. It was found that the concentration slip causes a nonlinear reaction rate distribution at large Damköhler numbers. The results also showed that an accurate prediction of the rarefied gas effect on catalytic reactions in microscale reactors has to consider both the temperature slip and the concentration slip.

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1. Introduction

The recent development in microfabrication technology has led to great interests in microscale combustion for power generation, chemical sensing, and fuel conversion. The research in microscale combustion has been motivated by the fact that hydrocarbon fuel has an energy density per unit mass (50 MJ/Kg) or volume that is 100 times more than the most efficient lithium-ion batteries (0.5 MJ/Kg). Furthermore, hydrocarbon fuel-based microcombustors also have the advantages of lighter weight, longer life time, immediate recharge, and less environmental impact than batteries. Moreover, microscale combustion also has higher thermal

efficiency than macroscale combustors due to the increased surface to volume ratio and heat recirculation. Despite the merits of microscale combustion, combustion in meso and micro scales yields challenges in understanding the impacts of heat loss, radical quenching, and non-equilibrium transport on homogeneous and heterogeneous combustion.

It is well known that with the decrease of the combustor scale, the increase of larger surface to volume ratios dramatically increases the wall heat loss and leads to flame extinction. On the other hand, the reduction of thermal inertia at small scale significantly reduces the response time of the wall and leads to strong wall flame coupling. This flame–wall interaction can dramatically change the nature of flame propagation in small scale devices. In particular, at small scale, the heat recirculation through the wall heat conduction yields new flame regimes and instabilities.

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Previous studies have shown that the wall heat loss results in the so-called quenching distance below which a flame cannot propagate (Williams, 1985). However, Weinberg and co-workers (Weinberg, 1971; Lloyd and Weinberg, 1975, 1976) studied the heat recirculation effects by reversing the burned gas to preheat the unburned mixture and their results showed that the flammability limit can be extended and that there are two limits caused by heat loss and flow rate, respectively. Theoretical analyses (Ronney, 2003; Ju and Choi, 2003; Ju and Xu, 2005) also predicted this observed phenomenon and demonstrated the existence of different flame regimes in mesoscale channels caused by this wall–flame thermal interaction. Numerical simulations (Norton and Vlachos, 2003; Leach and Cadou, 2005; Maruta et al., 2005) showed that it was possible to build microburners below the quenching distance with a proper choice of wall materials and reduced heat loss. Experimentally, a number of innovative ways have been devised to reduce thermal losses and build up micro combustors near or below the quenching distances, including the single pass (Peterson and Hatfield, 2001), the Y-shaped diffusion burner (Miesse et al., 2005) and the three-dimensional “Swiss Roll” (Sitzki et al., 2001; Ahn et al., 2004) counter flow heat-exchanger/combustor. A microburner with a scale of less than 1 mm has also been developed by Masel and Shannon (2001) to allow self-sustained homogeneous combustion, which is achieved by using certain insulated alumina to reduce radical adsorption and heat loss.

Industry and military applications require that the micro power generators be portable as well as efficient. However, with the channel width further decreased, it becomes very difficult to sustain a stable propagating flame due to the quenching effect of the wall and the requirement of high-operating and ignition temperatures of hydrocarbon fuels. On the other hand, catalytic combustion can take advantage of the high surface to volume ratio and high transport rate in microscale and generate enough radicals to sustain the reaction. This provides an opportunity for faster catalytic reactions than could be achieved with macroscale combustors. Many numerical simulations and experimental work have been conducted to study the ignition, stability and conversion efficiency of catalytic microburners (Ahn et al., 2004; Norton and Vlachos, 2005; Boyarko et al., 2005). Some catalyzed microburners have been built to achieve sustained catalytic microcombustion over a wide range of compositions and at substantially lower temperatures and pressures than macro combustors where traditional homogeneous combustion may not survive. All of these studies were focused on combustion in the continuum regime. The burner scales were so large ($> 100 \mu\text{m}$) that the rarefied gas effect was ignored.

However, when the length scale of the flow approaches the mean free path of the combustion mixture, there are no longer sufficient collisions between gas molecules to achieve thermodynamic equilibrium. For example, the mean free path of the partially burned methane–air mixture at 1000 K and one atmosphere is around $0.1 \mu\text{m}$. The resulting Knudsen number for microcombustion is between 0.001 and 1.

Norton et al. (2004) have developed catalyzed microburners that allow self-sustained combustion in channels with a gap of $250 \mu\text{m}$ and peak pressure of 5000 Pa within a temperature range of 800–1000 K, which yielded a Knudsen number of 0.02. As such, in microscale combustion, the resulting non-continuum and non-equilibrium transport processes cannot be well predicted without reasonably considering the rarefied gas effect.

Slip models accounting for velocity and temperature in micro fluidics have been developed and employed in the numerically efficient continuum methods to correct the non-equilibrium processes near solid boundaries (McNenly et al., 2003). The basic idea is to relax the traditional no-slip boundary to allow for the presence of slip on the surface while the equations applicable to the continuum regime are retained. It is well known that the temperature and velocity slips on the wall can greatly affect the energy exchange between the gas and the wall (Kavehpour et al., 1997). In a microscale combustor, these slips will also affect the catalytic surface reaction due to the strongly temperature dependent Arrhenius law and transport properties. A recent study of catalytic conversion in micro-channels has shown that slip flow significantly affects the conversion efficiency (Succi, 2002). Shankar and Glumac (2003) studied the temperature slip effect in a low pressure catalytic combustion system and they observed a slip of 34 K in the hydrogen/oxygen reaction system. Similar to the velocity and temperature, there is a possibility that the species concentration near the boundary may also be very different from that at the boundary (Rosner and Papadopoulos, 1996), which significantly influences the surface reaction. Raimondeau et al. (2002) and Aghalayam et al. (1998) numerically studied the role of radical wall quenching in flame stability and wall heat flux and their results showed that quenching of any of the important radicals had a significant influence on the stability of the system due to the chemical and thermal coupling between the gas and the wall. It has been shown that while the species concentration could be very uniform in a micro channel when the wall was inert, certain radicals could also have a large gradient of concentration near the reactive surface. This could have been the case especially if the reaction speed was larger than the transport speed (Aghalayam et al., 1998), which renders a possible large radical discontinuity between the gas and the wall. The rarefied gas surface reaction is also an important issue in chemical vapor deposition because many depositions are conducted at very low pressure environments. In spite of its great practical importance and the increasing interests in studying the velocity and temperature slips in microfluidics, the radical or species concentration slip and its impact on catalytic reactions in micro and nano scales have not been well investigated.

This study was motivated by the above discussion and was aimed to develop a slip condition of species concentration for the purpose of numerical modeling of micro and nanoscale chemical reactors. First, a concentration slip model was developed from the approximate solution of the Boltzmann

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