Studies of Slip Effects on Fuel Oxidation in Microscale Catalytic Reactors

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Introduction

The importance of slip effects in modeling heterogeneous combustion systems such as catalytic combustion and combustion synthesis of thin films at small scales is gaining more and more attention. It is known in rarefied gas flows [1,2] that, under conditions of large Knudsen numbers, both species and temperature slips are present at the gas-surface interface. The effect of temperature slip in low pressure catalytic combustion systems was investigated experimentally [3]. The results showed that the temperature slip was about 34K at a pressure of 2.5 Torr, which had a very significant effect on the methane oxidation.

The slip effects in low pressure or micro scale systems tend to affect the reactivity in different ways. The non-equilibrium effects near the wall intend to reduce the mass and energy transport processes, which will cause species concentration and temperature discontinuity. Firstly, the gas species mole fraction at the wall can change due to slip. The species slip, especially the radicals slip at the catalytic wall will significantly affect gas phase radical distributions as well as the gas phase reactions. Secondly the reaction rates of the systems can be greatly affected by temperature jump due to the high dependence of temperature. Furthermore, the temperature jump will also affect the transport phenomena because of the moderate dependence of some of the transport coefficients on temperature. The slip effect, especially the species slip on surface reaction has not been well understood so far and further work need to be done.

Current work

In this work, the coupling between the surface catalytic reactions and the homogeneous gas phase reactions in a microscale catalytic channel is investigated using the slip boundary conditions developed in [2]. A two-dimensional code integrated with CHEMKIN and SURFACE CHEMKIN is developed to study the rarified gas effect. The premixture flows into the channel with uniform velocity, concentration and temperature profiles. Three different types of nonequilibrium effects (temperature, velocity and species slips) are considered at the catalytic surface. The calculation domain is shown in Fig. 1.

Conclusion

The results show that the rarefied gas effect significantly reduces the momentum, heat, and mass transfer near the wall, and thus decreases the surface reaction rate. Furthermore, it is shown that the slip effects can dramatically change some radical distributions, which will yield a strong coupling between the gas phase reaction and catalytic surface reaction in microscale reactors. It also shows that the temperature jump has an opposite effect when the gas temperature is higher or lower than the wall temperature. Finally, there is a nonlinear distribution of surface reaction rates near the entrance of the microchannel resulted from the slip effects shown in Fig. 2. And also the surface reaction rates of major species can be reduced by the slip effects.

Fig. 1 Sketch of the microscale catalytic channel

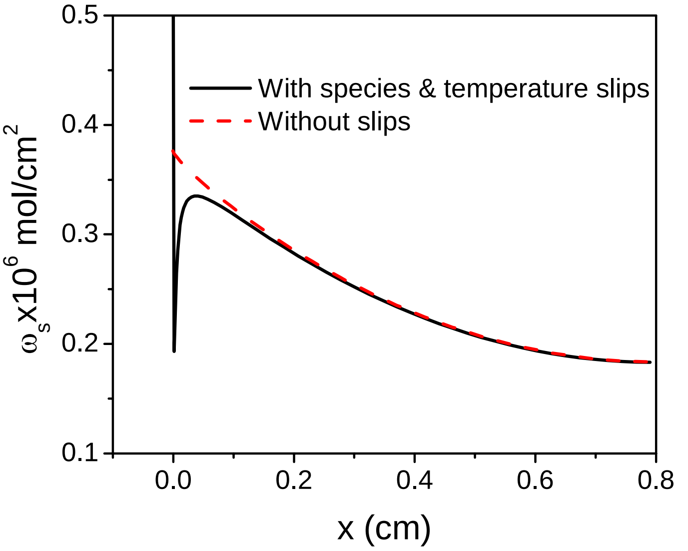

Fig. 2 Surface reaction rate of methane (T_w=1200K)

Reference

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