Numerical Simulation of Hydrogen/Air Combustion Characteristics inside a Platinum Micro Tube

Guan-Bang Chen[1], **Yei-Chin Chao**[2], **Chih-Peng Chen**[2], **and Chih-Yung Wu**[2]

[1] Department of Cmputer Science and Information Engineering,
Diwan College of Management
87-1, Nansh Li, Madou Jen. Tainan, Taiwan, 721, ROC
[2]Institute of Aeronautics and Astronautics, National Cheng Kung University
Tainan, Taiwan, 701, ROC

Introduction

Studies of combustion in a micro-scale reactor for micro-power generation and micro-propulsion systems are receiving intensive attention and interest recently [1]. For power generation, combustion usually can produce much higher power density than conventional Lithium batteries. In addition, it can provide longer operational cycles and reduce the mass and volume fraction of the power system. Besides, micro-scale combustion can also be used in the micro thruster for micro and pico satellites and micro combustors may be designed by using MEMS technologies.

When the size of the conventional reactor is reduced to sub-millimeter scales, losses of heat and chemical radicals through wall surface significantly affect the combustion behavior, and to maintain intensive reaction (combustion) in a micro combustor becomes a difficult practice. Combustion will quench when the size of the combustor is reduced smaller than the quenching distance or diameter. Probable factors of quench in a micro combustor include: higher surface-to-volume ratio, enhanced radical depletion on the wall, and keener competition of different time scales. In order to reduce heat loss due to high surface-to-volume ratio, many creative designs such as, "Swiss roll" combustor and heat-recirculating combustor are proposed [2,3]. Furthermore, catalyst was also used to enhance the reaction in low temperature and lean reactions and to reduce radical depletion on the wall [4-6]. Being limited by the size, it is very difficult to obtain information inside a micro reactor by systematic experimental studies. Numerical simulation plays an important role in micro-combustion studies. Some numerical studies showed the influences of heat transfer and flow field on the reaction inside micro-channels [7-9]. However, most of the studies concentrated on the surface or gas phase reactions separately. In order to simulate the mutual interaction of gas phase and surface reactions inside an actual catalyst channel, a two-dimensional CFD model of a micro tube with multi-step gas phase and surface reactions for H_2/air mixture is solved in this work.

Numerical Method

In this work, numerical simulation for an axisymmetric cylindrical channel flow with gas-phase and catalytic surface reactions is performed. The numerical model consists of the Navier-Stokes equations, mass and energy conservation equations and species equation for each chemical species. The schematic computational domain and boundary conditions are shown in Fig. l. The diameter of the tube is $1000\mu m$, $500\mu m$ or $200\mu m$ and the length is 1cm.

Uniform wall temperature is specified since platinum has high thermal conductivity. High thermal conductivity will enhance upstream transfer of heat through the wall and result in more uniform wall temperature [10]. Non-uniform mesh is used in this work and more grids are distributed in the reaction region. The uniform flow condition is specified at the inlet for all variables. At the exit, the pressure is specified and an extrapolation scheme is used for species and temperature. Muti-steps reaction chemistry is used in the gas phase and on the surface. The gas-phase reaction mechanism composes of 9 species and 20 reaction steps which are adopted from the literature [11]. The surface reaction mechanism has been compiled primarily from the work of Deutschmann et al. [12] and has been tuned for catalytic ignition of H_2. The Chemkin software for gas-phase chemical kinetics and Surface Chemkin for heterogeneous chemical kinetics are used in this study.

Results and Discussion

In this work, the effects of different operational parameters on hydrogen/Air combustion characteristics inside a platinum micro tube are performed by numerical simulation. Especially, the interaction of gas phase reaction and surface reaction inside the platinum tube is discussed. The parameters studied are the inlet velocity (residence time), fuel equivalence ratio, tube diameter and wall temperature. At lower wall temperatures (1200K and below), all the simulation results show that the flow is dominated by surface reaction. This can be identified by OH concentration contours where the highest OH concentration is on the surface. At low temperatures, different parameters will change the transition location from kinetic control to diffusion control regions. Figures 2 to 5 show the fuel concentration at the wall as a function of inlet velocity, fuel equivalence ratio, tube diameter and wall temperature, respectively. The transition location from kinetic control region to diffusion control region will shift downstream with increasing inlet velocity due to decreasing residence time. It will also shift downstream with increasing fuel equivalence ratio and tube diameter. However, it will shift upstream with increasing wall temperature due to the increasing velocity and decreasing residence time near the wall (see Fig. 5). At high temperatures, gas phase reaction will occur inside the tube and its location will shift upstream with increasing inlet fuel concentration. Figure 6 show the OH contours as a function of inlet velocity inside a 500 μ m platinum tube. The location of gas phase reaction will shift downstream and approaching the wall at the exit with increasing inlet velocity. When the inlet velocity exceeds a critical value, the gas phase reaction can not be maintained at the exit and the flow is dominated by surface phase reaction. As the tube diameter decreases, gas phase reaction is inhibited due to the enhanced diffusion to the wall (see Fig.7). For this case, the flow is domination by surface reaction and gas phase reaction will occur only in the case of an equivalence ratio of 1.0 and a wall temperature of 1500K.

Conclusions

Numerical simulation of H_2/air mixture reaction in a Pt catalytic micro tube is performed to identify the effects of different operational parameters on the interaction of gas phase and surface reactions inside the tube. When the flow is dominated by surface reaction, different parameters primarily affect the transition location from kinetic control region to diffusion control region. At high temperatures, when gas phase reaction can occur inside the tube, variation of the operational parameters will affect the light-off location of gas phase reaction. The location of gas phase reaction will shift downstream with decreasing equivalence ratio or

increasing inlet velocity until the gas phase reaction can not be maintained at the exit. During this process, the surface reaction dominates the upstream flow region and extends downstream with increasing the inlet velocity and finally all over the tube. Decreasing the tube diameter will enhance the fuel diffusion and heat loss and inhibit the gas phase reaction to limited cases of near stoichiometric and very high wall temperatures.

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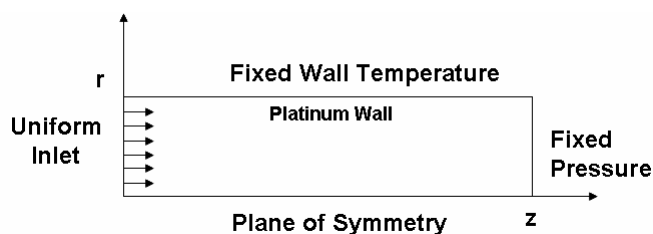12. Deutschmann, O., Schmidt, R., Behrendt, F., an *Institute*, 26:1747-1754 (1996).

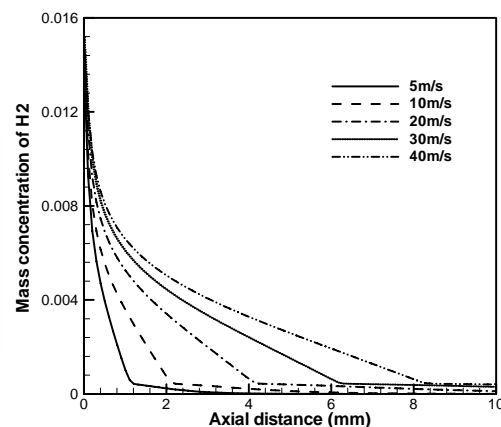Figure 1 schematic of computational domain

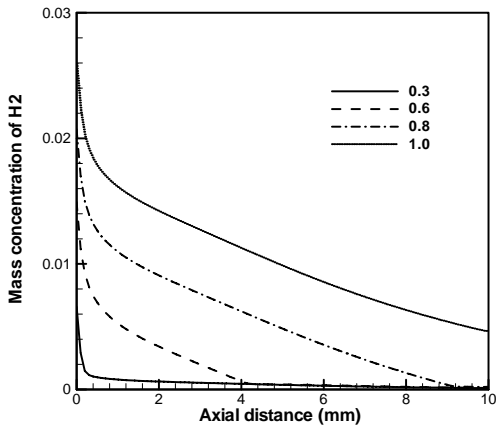Figure 2. H_2 concentration at the wall as a function of inlet velocity in a 500 μ m Pt tube, T_w=1200K , ϕ =0.6

Figure 3. H$_2$ concentration at the wall as a function of equivalence ratio in a 500 μ m Pt tube, T$_w$=1200K, velocity=20m/s
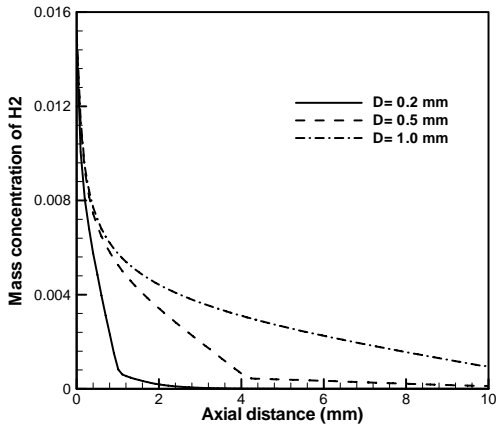

Figure 4. H$_2$ concentration at the wall as a function of tube diameter at a velocity of 20 m/s, T$_w$=1200K , ϕ =0.6
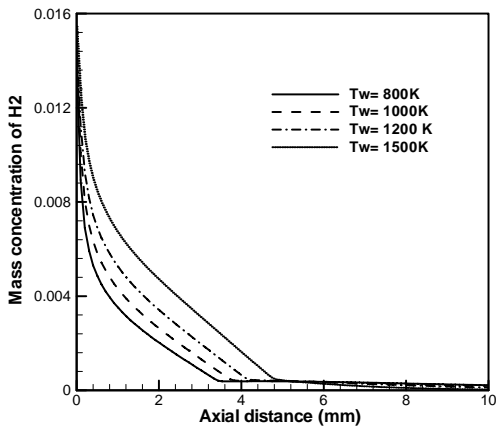

Figure 5. H$_2$ concentration at the wall as a function of wall temperature in a 500 μ m Pt tube, ϕ =0.6 , velocity=20m/s
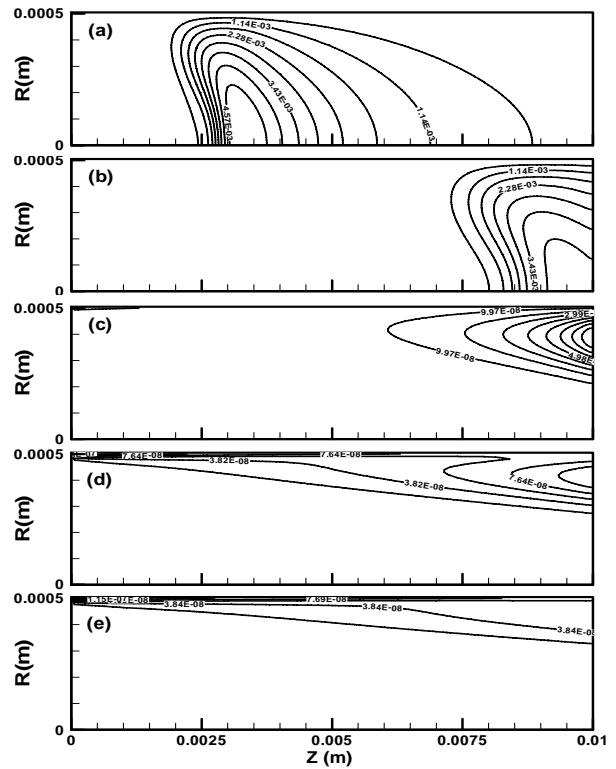

Figure 6. OH concentration inside a 1000 μ m Pt tube (ϕ =0.8, T$_w$=1500K, a-e: V=5,10,20,30,40 m/s)
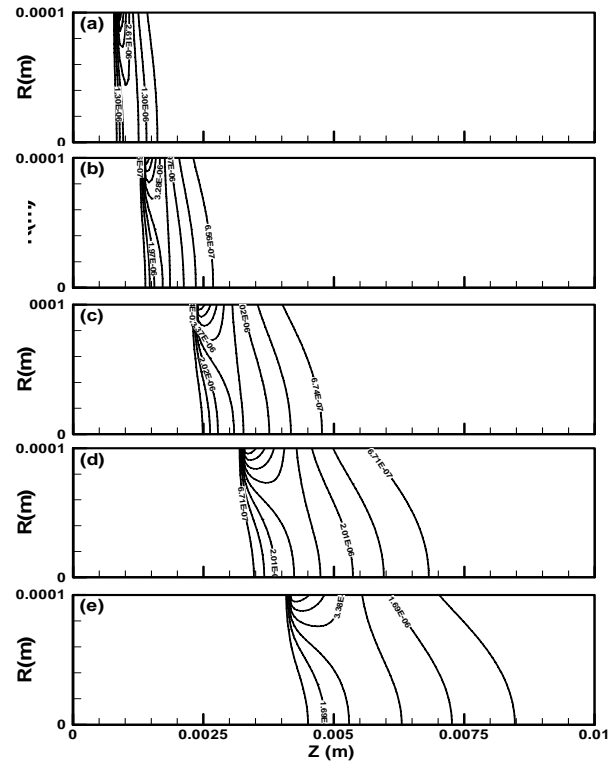

Figure 7. OH concentration inside a 200 μ m Pt tube (ϕ =0.8, T$_w$=1500K, a-e: V=5,10,20,30,40 m/s)