Numerical Modeling on the Flow Characteristic of Catalytic Combustion Over a 2D Cylindrical Bluff Body

Chih-Yung Wu[1], Ching-Ching Cheng[1], Yung-Sheng Lien[2]
[1]Department of Mechanical and Automation Engineering, Kao Yuan University
Kaohsiung, Taiwan, ROC

[2]Advanced Engine Research Center, Kao Yuan University
Kaohsiung, Taiwan, ROC

1 Introduction

Due to energy depletion and the environmental issues, it is significant to use energy with high efficient systems. The interest in micro-combustors mainly stems from the increasing demands for micro power generator systems and portable devices especially for electronical consumer devices or military application [1]. It has been well known that the catalytic combustion has been studied for several decades [2]. It is an efficient way to burn fuels in premixed mixtures with less emissions at low reaction temperatures. The catalytic combustion technique can also be applied to the meso- and micro- scale combustion for portable power sources [3], ultra-lean oxidation [4] and ultra-rich partial oxidation of fuels to produce hydrogen [5] and syngas oxidation for heat recovery.

Traditionally, the catalytic reactor can be composed of carriers, active components, and monolithic substrates or a tubular chamber filled with catalytic ceramic beads. However, higher pressure drop occurs as the mixture flow through the traditional catalytic reactor. Recently, the modification of the reactor geometry for catalytic reaction enhancement have been proposed [7][8]. Moreover, the active wire meshes can also be used for catalytic combustion [9]. The wire can be regarded as a bluff body. As mixtures flows past a bluff body, vortices are created at the back of it and detach periodically from either side of the bluff body. The motivation behind the current research is how to determine the concise design to fabricate the portable power device with low pressure loss catalytic reactor. How a single cylinder or wire with catalytic surface promotes oxidation reactions in the flowfield? Does vortex shedding at the downstream of wire of cylinder affect conversion ratio of catalytic reaction? To address these questions, the investigation on the flow near catalytic surface and boundary layer phenomena is necessary. Objectively, the purpose of this paper is to present a numerical study on the flow characteristic of catalytic combustion over a 2-D cylindrical bluff body.

Correspondence to: chihyungwu@gmail.com

2 Methodologies

The time-dependent governing equations of continuity, momentum, energy, and chemical species are solved using the commercial package CFD-ACE+ 2014.0 coupled with chemical kinetic mechanisms from Miller and Bowman [10]. The molecular transport and thermal data are obtained from the CHEMKIN package; the code then computes the thermal conductivity and viscosity of the mixture using Wilke's formula. The transient calculations with a time step $\triangle t = 10^{-4}$ sec was applied. In the present study, the backward Euler method was used for the temporal differencing. An non-uniform staggered-grid system is used with a control volume formulation in accordance with the SIMPLEC algorithm, which is shown schematically in Fig. 1.The inlet conditions are specified as fixed velocity at the inflow boundary of the computational domain. Fixed pressure boundary conditions are imposed on the open boundaries of the exit. The transport model also includes thermal diffusion to account for species diffusion due to temperature gradients. The total number of grids was 301 in the vertical direction and 502 in the axial direction for a computational domain of 40 mm×50 mm with a minimum grid spacing of 0.1 mm. The minimum grid size was used near the central axis and the 2D cylindrical bluff body, and an enlarged grid size was used close to the outer boundaries. The surface of the 2D cylindrical bluff body was set as catalytic surface, and the reaction mechanism was compiled primarily from that proposed by Deutschmann et al [11]. Convergence of the solution was declared when the ratio of the change of the dependent variables to the maximum variables in that iteration was less than 1×10^{-4}. The research condictions including eqvalence ratio, inlet velocity(U), Renolds number(Re_d) that is the ratio of inertial to viscous forces around the 2D cylindrical bluff body, Strouhal number(St) as well as the theoretical vortex shedding frequency (f) that calculated using eq. (1) are listed in Table 1. The initial conditions of flow in the computation domain were set as uniform flow velocity and equal to the inlet velocity. In order to ignite the reaction and evaluate the final result of characteristics of reacting flow quickly, the initial conditions of temperature of 2D cylindrical bluff body were set as the equilibrium temperature of the mixtures.

$$St = 0.198\left(1-\frac{19.7}{Re_d}\right) = \frac{f\cdot d}{U} \quad (1)$$

3 Results and Discussion

The calculated vortex shedding frequencies compared with the theoretical values those estimated using eq. (1) with different Reynolds number for cold flow without chemical reaction was examined and shown in Fig. 2. The results show that the numerical simulation can predict the vortex shedding frequency precisely. Note that the frequency is monitored at 10 mm downstream of the 2D cylindrical bluff body, and the power spectrums are calculated using Fourier transform. Fig. 3 shows the transient evolution of vortex shedding in terms of temperature for four cased labeled in Table 1. Fig. 3 shows the ignition transient evolution of vortex shedding in terms of temperature for case #1. At beginning, the reaction occurs near catalytic surface, and the reaction products as well as the hot gas flows downstream and forms a symmetry vortex pair. In a continuous flow the instability occurs when a velocity shear is exist. Hence, the Von Kármán vortex sheet can be found. Similar phenomena can also be found for case #2 and #3 which are shown in Fig. 4 and Fig. 5, respectively. For lower equivalence ratio, the gas phase reaction or flame cannot be formed. As shown in Fig. 6, the surface reaction occurs near catalytic surface initially, and the reaction products also forms a symmetry vortex pair. However, as $t = 1.6 \times 10^{-3}$sec, the gas phase reaction is ignited. As the gas phase reaction is formed, the Von Kármán vortex sheet cannot be found. The vortex shedding frequency was calculated numerically and shown in Fig. 7(a). For the cases that gas phase reaction cannot be ignited, the vortex shedding frequency is approximate to theoretical value that calculated based on Reynolds number. In addition, as the gas phase reaction occurs, the Von Kármán vortex cannot be found. On the other hand, the conversion ratio which are defined as eq. (2) are shown in Fig. 7(b). It can be found that the conversion ratio is increased as the equivalence ratio is increased, and the conversion ratio increases dramatically as the gas phase reaction is ignited.

$$\mathrm{CR} = \frac{\sum_{in} \dot{m}_{H_2} - \sum_{out} \dot{m}_{H_2}}{\sum_{in} \dot{m}_{H_2}} \times 100\% \qquad (2)$$

4 Conclusions

In the present study, the flow characteristic of catalytic combustion over a 2D cylindrical bluff body has been numerically studied. Generally, the Von Kármán vortex sheet can be found at the downstream of 2D cylindrical bluff body. The vortex shedding frequency is dominated by the Reynolds number. The conversion ratio can be increased as the gas phase reaction is ignited and sustained in the flow field.

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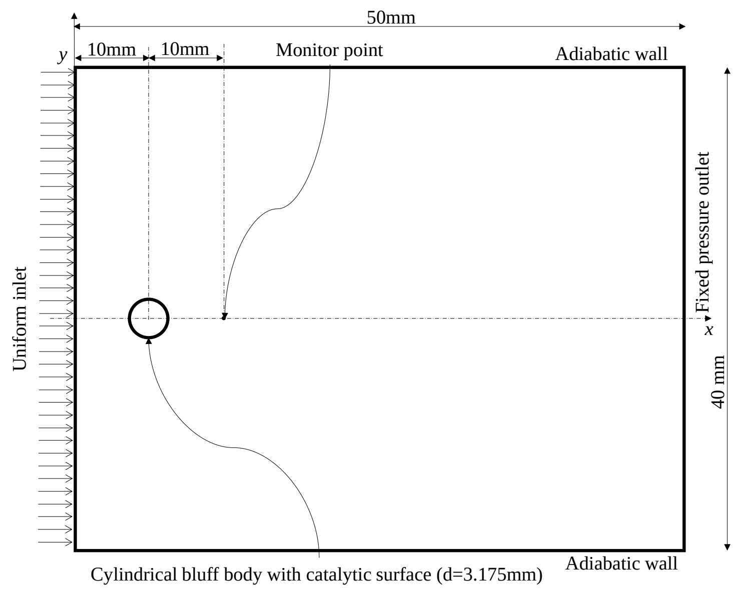

Figure 1. Computation domain with boundary conditions

Table 1: The research conditions

Case	ϕ	T_{ad}(K)	U(m/s)	*Re*	*St*	f_t (Hz)
1	0.1	631.53	0.6	1,151.54	0.195	367.772
2	0.2	926.27	0.6	1,111.37	0.194	367.541
3	0.3	1,189.7	0.6	1,074.33	0.194	367.312
4	0.4	1,428.5	0.6	1,040.19	0.194	367.087

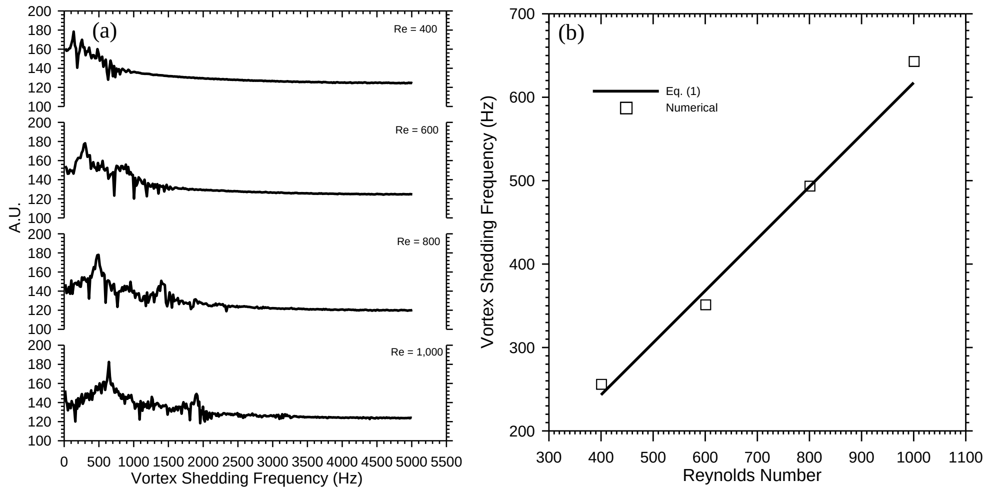

Figure 2 The vortex shedding frequencies with different Reynolds number for cold flow: (a) power spectrum; (b) comparison between theoretical and numerical predicted values

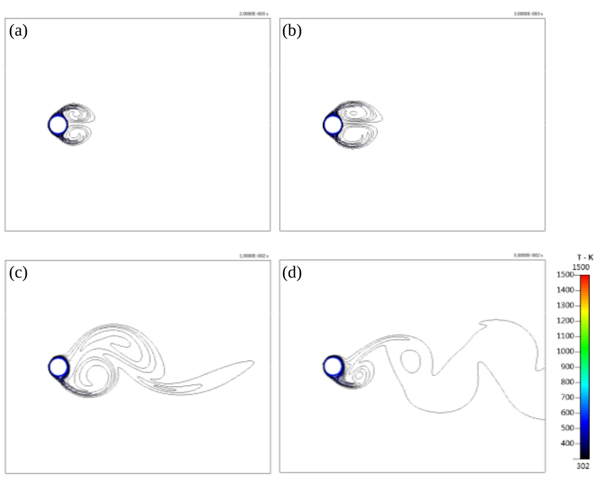

Figure 3 The transient evolution of vortex shedding in terms of temperature for case #1：(a) $t = 2\times10^{-3}$ sec; (b) $t = 3\times10^{-3}$ sec; (c) $t = 1\times10^{-2}$ sec; (d) $t = 5\times10^{-2}$ sec

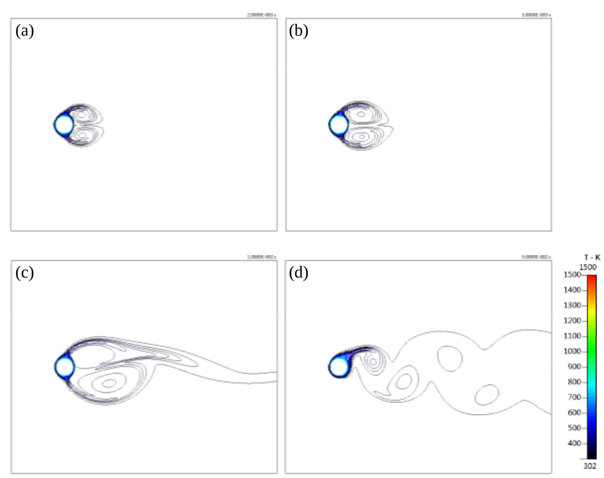

Figure 4 The transient evolution of vortex shedding in terms of temperature for case #2：(a) $t = 2\times10^{-3}$ sec; (b) $t = 3\times10^{-3}$ sec; (c) $t = 1\times10^{-2}$ sec; (d) $t = 5\times10^{-2}$ sec

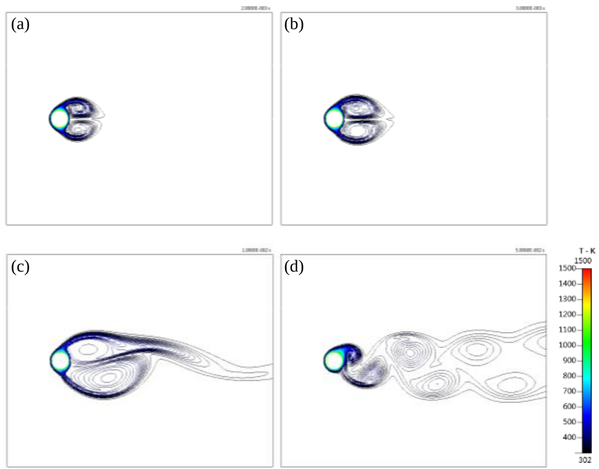

Figure 5 The transient evolution of vortex shedding in terms of temperature for case #3 : (a) $t = 2\times10^{-3}$ sec; (b) $t = 3\times10^{-3}$ sec; (c) $t = 1\times10^{-2}$ sec; (d) $t = 5\times10^{-2}$ sec

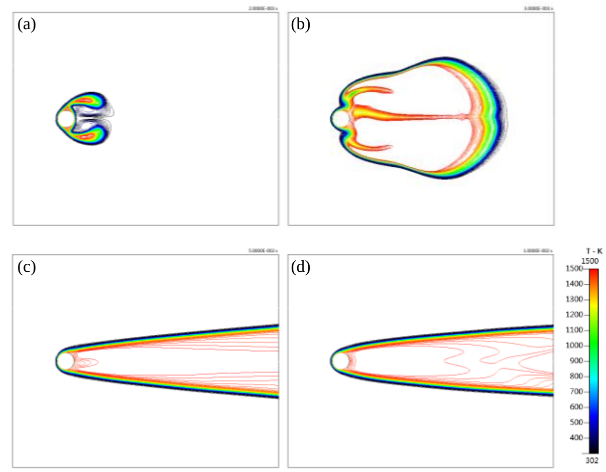

Figure 6 The transient evolution of vortex shedding in terms of temperature for case #4 : (a) $t = 2\times10^{-3}$ sec; (b) $t = 3\times10^{-3}$ sec; (c) $t = 1\times10^{-2}$ sec; (d) $t = 5\times10^{-2}$ sec

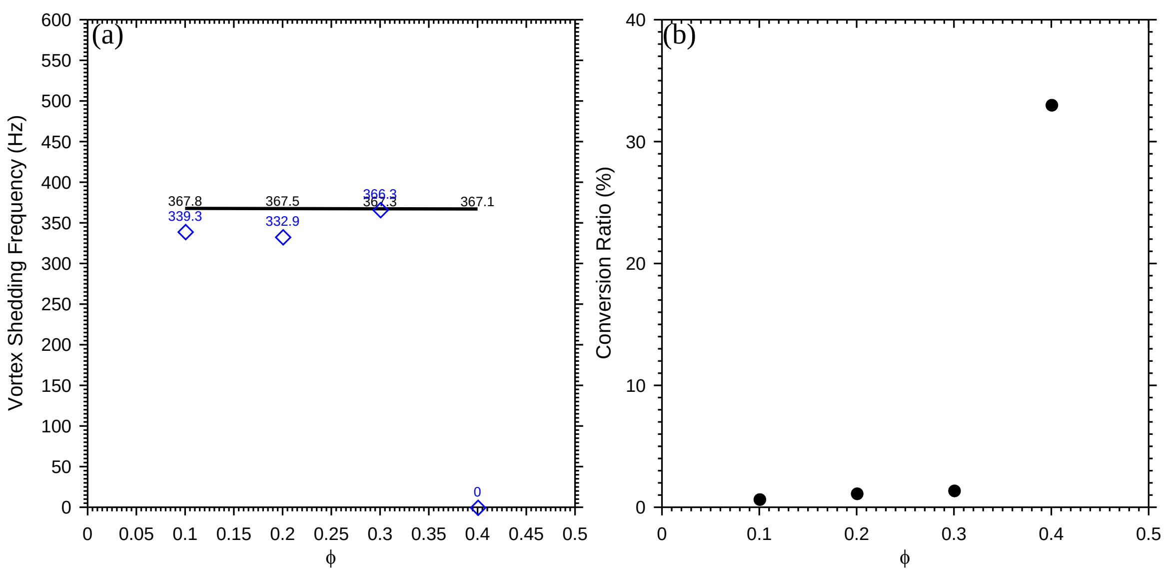

Figure 7 Vortex shedding frequency and conversion ratio for four cases

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