

Chemical Effects on Turbulent Premixed Flames nearby a Wall Surface

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1 Introduction

Since the middle of the 20th century, it has been required to be the enhancement of energy efficiency and the reduction of emission with environmental load for actual combustors such as the engines of automobiles, ships and airplanes. For design of the engines, it is necessary to understand the conditions of flow and combustion in engine cylinder in detail and to predict them precisely. In engine cylinder, turbulent flames mainly occurs, hence to investigate their detailed structure quantitatively, it is effective to utilise high accuracy database constructed by DNS. Numerical simulations such as RANS and LES are often used for the development and design of engines recently. Many turbulent combustion models used in their simulations have been developed, however chemical processes on the wall surfaces of combustors are not considered in any current models. For example, in the engine cylinder for automobiles, very narrow space is surrounded by metal walls such as cylinder liner, cylinder head, piston, etc. around top dead centre compression stroke, hence it is easy to imagine that the influence of metal walls on the combustion occurred in the vicinity of the walls is not negligible. Therefore chemical processes on the wall surface should be considered to investigate the condition of combustion in engine cylinder exactly. Any numerical works considered surface reactions on the wall surface are implemented in one dimension by Popp et al. [1], Rinnemo et al. [2], Fernandes et al. [3] or in two dimension with turbulent model by Mantzaras et al. [4], there are no studies in two or three dimensional DNS. Under no consideration of surface reactions, recently, the behaviours of turbulent premixed flames near walls were discussed in detail by using three dimensional DNS by Tsunemi et al. [5]. In the present study, two dimensional DNS of turbulent premixed flames was conducted with chemical processes on the wall surface, and the influence of chemical processes and adsorbates on the walls on turbulent premixed flames were discussed.

2 Numerical scheme and conditions

The target in the present study is a hydrogen/air turbulent premixed flame under the flow field in the parallel plates. The computation is implemented in a 4 mm × 4 mm square domain with 256 × 256 grid points resolution. Numerical conditions are shown in Table 1. ϕ denotes equivalence ratio, u_L^0 laminar

burning velocity without flame stretch, p_∞ pressure at infinity, Le Lewis number of deficient species (in the present case, hydrogen). The governing equations are two dimensional compressive Navier-Stokes equation, mass and species conservation equations, and energy conservation equations. 6th order compact finite difference scheme by Lele [6] is used for spatial discretisation, 3rd order Runge-Kutta method for time advancement. Non-reflective inflow condition and outflow condition based on NSCBC (Navier-Stokes Characteristic Boundary Condition) [7] is applied for the upstream and downstream boundary respectively, and non-reflective adiabatic non-slip wall condition is applied for lateral boundaries. For gas phase reactions, hydrogen/air detailed chemical mechanism with 9 species and 35 elementary reactions by Stahl and Warnatz [8] is used, for chemical processes on the wall surface, hydrogen/oxygen surface reaction mechanism with 4 adsorbates and 13 elementary reactions by Williams et al. [9] is used. The assumptions for chemical processes on the wall surface are as follows:

- Langmuir adsorption model
 - Langmuir-Hinshelwood mechanism
- Adsorption rate is described by Langmuir rate equation

$$k_{a_i} = \frac{s_i}{(2\pi M_i RT_g)^{1/2}}, \quad (1)$$

desorption rate is described by Arrhenius rate equation, where k_{a_i} denotes adsorption rate constant of species i , M_i molecular weight of species i , R gas constant, T_g temperature of gas phase, s_i sticking coefficient of species i .

- Langmuir competitive adsorption model
- Ignore the interaction other than the reaction between adsorbates.
- As for mass diffusion from gas phase to wall surface, diffusion velocity is described by Stefan velocity

$$V_{D_i} = \frac{\dot{\omega}_i M_i}{\rho Y_i} - u_s, \quad u_s = \frac{1}{\rho} \sum_{i=1}^{n_g} \dot{\omega}_i M_i \quad (2)$$

in the direction normal to the surface, and is ignored in the direction parallel to the surface [10], [1], where V_{D_i} denotes diffusion velocity in the direction normal to the surface of species i , ρ density, Y_i mass fraction of species i , $\dot{\omega}_i$ production rate of species i , n_g number of species in gas phase.

- Ignore the diffusion velocity of adsorbates.

The calculation in the present study was implemented by Super Computer NEC SX-8R and SX-9, Large-Scale Computing System, Cybermedia Center, Osaka University.

Table 1. Relevant numerical conditions.

ϕ	uL^0 [m/s]	p_∞ [MPa]	Le	u' [m/s]	L [mm]	Re_λ
0.7	0.8364	0.101325	0.4308	0.528	3.44	56.7

3 Results and discussion

In our previous study, it was found that for laminar flames without surface chemistry a flame is attached on the wall and spreads along the wall without quenching, while with surface chemistry a flame quenches without attaching on the wall and does not spread as shown in Fig. 1 [11].

The distributions of temperature and heat release rate of turbulent premixed flames with chemical processes nearby the walls are shown in Fig. 2. Turbulent premixed flames are indicated by the distribution of heat release rate. The close-up views of the distributions of temperature and heat release rate near the centre of the lower wall are shown in Fig. 2. The turbulent flame is quenching although the wall surface is specified as an adiabatic condition. Around the wall near the quenching region, the increases of temperature and heat release rate are not observed, while in the region that heat release

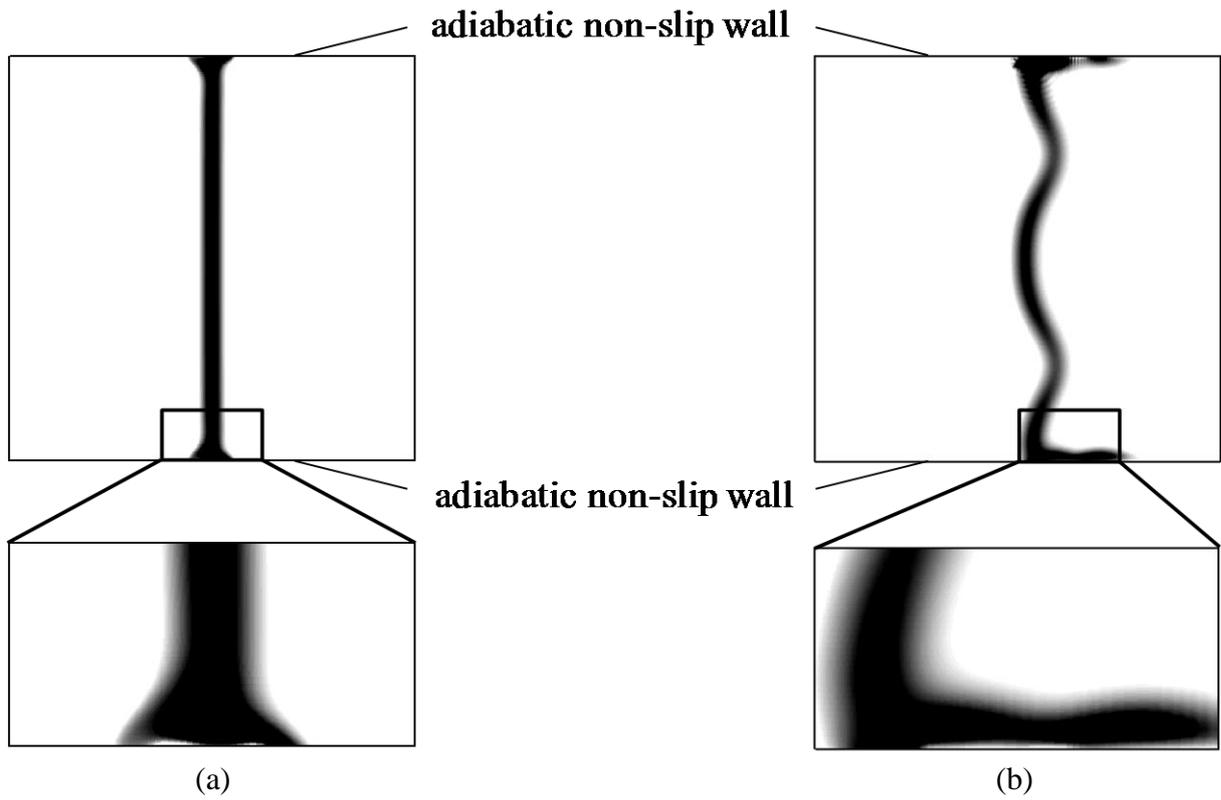


Figure 1. The distributions of heat release rate of laminar premixed flames (a) without and (b) with chemical processes near the walls.

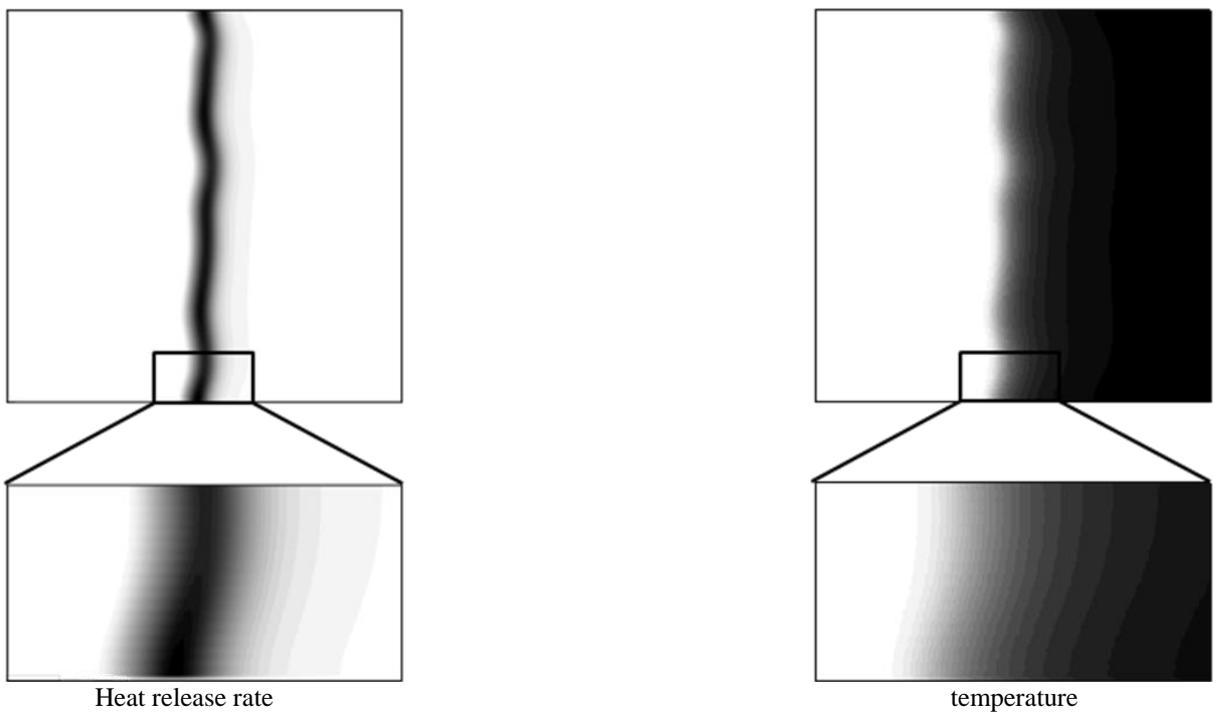


Figure 2. The distributions of heat release rate and temperature of turbulent premixed flames with chemical processes near the walls.

rate declines drastically, the drastic decrease of temperature is not observed. However, under the present conditions, it is necessary to consider the case of further developed turbulent flames.

The distributions of mole fraction and reaction rate of each adsorbate are shown in Fig. 3. These distributions are the close-up views near the centre of the lower wall, and the distribution of heat release rate is also shown to indicate the relative position of each adsorbate to the turbulent flame. The vertical axis is enlarged twice to make it easier to see them. O, OH, H₂O adsorbates inhabit in the upstream of the turbulent flame, while H adsorbate inhabits in the upstream and around the turbulent flame. OH adsorbate is consumed by chemical reaction around the upstream edge of the turbulent flame, while O, H₂O, H adsorbates disappear from the wall surface for reasons other than chemical reaction.

Therefore, the turbulent flames quench not due to the thermal conditions of the wall but to be the absences of most of adsorbates as important intermediates for the initiation and progress of chemical reactions on the wall surface.

4 Summary

Two dimensional DNS of turbulent premixed flames with chemical processes on the wall surface was conducted. The turbulent flame is quenching although the wall surface is specified as an adiabatic condition. In the region that heat release rate declines drastically, the drastic decrease of temperature is not observed, while most of adsorbates as important intermediates for the initiation and progress of chemical reactions are absent on the wall surface. Under the present conditions, the turbulent flame near the wall surface with chemical processes is influenced not by the thermal conditions of the wall surface but by the existences of some adsorbates on it.

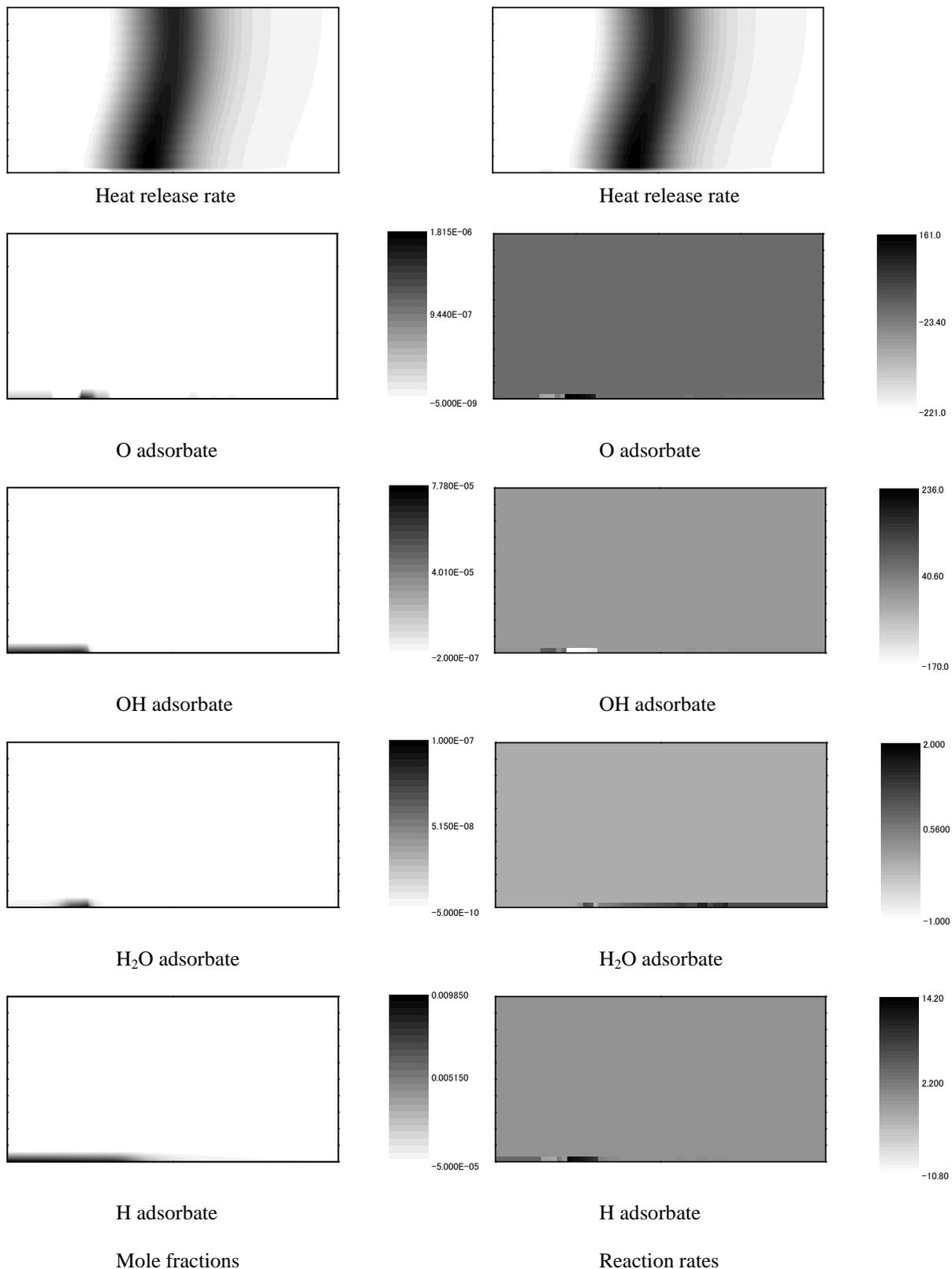


Figure 3. The distributions of mole fraction and reaction rate of each adsorbate around the centre of the lower wall.

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