Numerical Estimation of Ignition Conditions on Boundary Layer Combustion with Chemical Reaction Model

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The interest in hybrid propulsion is now growing in application to spacecraft propulsion and space transpotation. One of the attractive features of this technology is safety, which is important in space tourism industry.

In usual hybrid rocket engines, solid fuel is contained in combustion chamber into which liquid oxidizer is injected. The mixture of gasified fuel and oxidizer combust in the boundary layer over the fuel surface (Fig.1). Polypropylene and liquid oxygen, for example, are used as solid fuel and liquid oxydizer respectively.[1]

In order to realize a practical hybrid rocket, high rate fuel gas generation has to be achieved. Various studies have been performed such as low-melting point fuels and innovative oxidzer injection. To understand these methods closely, modeling and understanding of the mechanism, including fuel gasification, mixing of fuel and oxidizer, and turblent combusting flow, is necessary.

Although there are lots of studies performed on these themes, most of them consider the rate of reaction as infinity. However, because of the boundary layer combustion, the time scale of chemical reaction can be comparable to that of flow during ignition and extinction. Here Fig.2 shows that the "ignition time" can be sufficiently large in low temperature and low pressure conditions, which can be occured during ignition and extinction. In this paper, "ignition time" is defined as the time needed for 0-dimensional homogeneous reactants to reach a specific high temperature from when they appear suddenly at $t = 0$, on adiabatic and constant volume conditions. From this result, dismissing unsteadiness of chemical reaction can result in the failure of modeling ignition and extinction of hybrid rocket engine.

There is a tool "KUCRS[3]" that generates a list of elementary reactions and necessary various coefficients from a set of reactants. However, when this detailed reactions are included into fluid dynamics computation directly, the calculation cost will be too large for a practical use. Therefore we are trying to reduce the chemical reaction model. Fig.3 and Fig.4 show comparisons of results of propylene-oxygen combustion. Although the reduced reaction model uses 1/2 species and 1/4 elementary reactions compared to the detailed reaction model, good results are obtained in wide ranges of initial pressure, temperature and equivalence ratio.

In this paper, two themes will be discussed: one of them is chemical reaction reduction, and the other is numerical estimation of ignition conditions on boundary layer combustion, which imitates a hybrid rocket engine chamber, using this reduced reaction model.

For reduction of chemical reactions, the method above will be discussed. This method uses a sensitivity analysis and can be carried out without using special chemical knowledge such as classification of elementary reactions. In addition, futher reduction will be carried out via the concept of rate-controlled constrained equilibrium.[2] This method can reduce computational cost not only of chemical reaction calculation but also of chemical species mass conservation equations of fluids dynamics, without reducing the number of species used.

For numerical estimation of "ignition conditions" on boundary layer combustion, two-dimensional compressible fluid-dynamics equation where the chemical reaction model discussed above is engaged will be used. In this paper, "ignition conditions" means the conditions which various parameters, such as the initial temperature, the initial pressure, the amount of heat and the injection velocity of oxydizer, have to meet to let the reactants keep burning by themselves after an ignition process. The ignition time discussed above has relation to these ignition conditions because if the ignition time is large, much time will be needed for the reactants to ignite and generate heat, which is necessary for other reactants to react. The schematic of computational region will be similar to Fig.1, which images the surface of the solid fuel of a hybrid rocket. The ignition condition will be estimated numerically by changing the various parameters and the influences of them will be discussed. The influence of the unsteadiness of chemical reactions will also be discussed.

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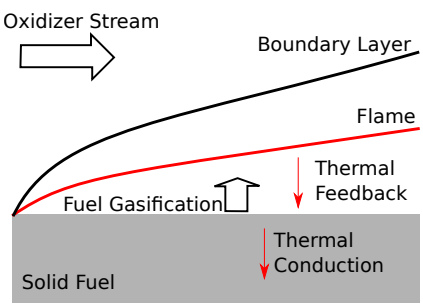

Figure 1: Schematic of combustion at hybrid rocket engine

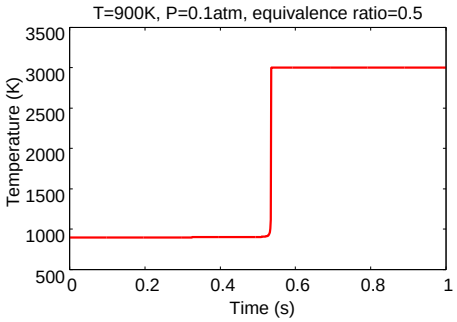

Figure 2: Calculated temperature change at low temperature, pressure and equivalence condition

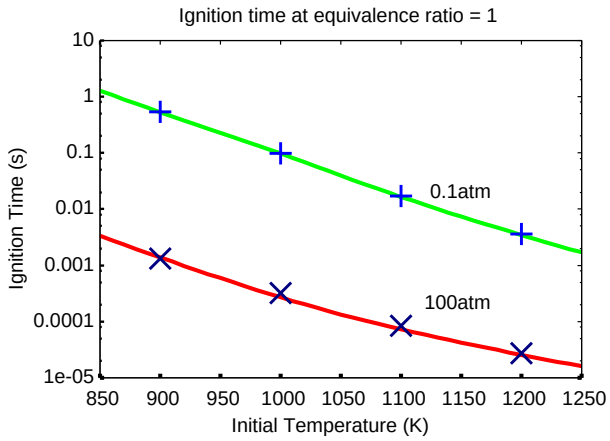

Figure 3: Comparison of ignition times of detailed model(cross) and reduced model(line) at equivalent mixture ratio

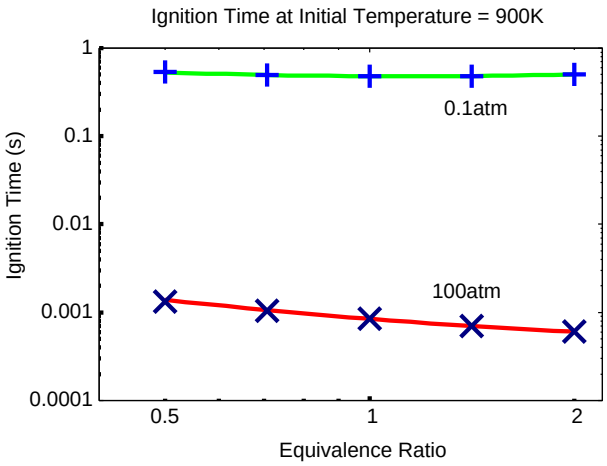

Figure 4: Comparison of ignition times of detailed model(cross) and reduced model(line) at a constant initial temperature

References

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[2] JAMES C. KECK. Rate-controlled constrained-equilibrium theory of chemical reactions in complex systems. *Progress in Energy and Combustion Science*, 16:30, 1990.

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