Hybrid Rocket Performance Prediction with Coupling Method of CFD and Thermal Conduction Calculation

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The final purpose of this study is to develop a design tool for hybrid rocket engines. This tool is a computer code which will be used in order to investigate rocket performance characteristics and unsteady phenomena lasting through the burning time, such as fuel regression or combustion oscillation. When phenomena inside a combustion chamber, namely boundary layer combustion, are described, it is difficult to use rigorous models for this target. It is because calculation cost may be too expensive. Therefore simple models are required for this calculation. In this study, quasi-one-dimensional compressible Euler equations for flowfields inside a chamber and the equation for thermal conduction inside a solid fuel are numerically solved. The energy balance equation at the solid fuel surface is solved to estimate fuel regression rate. Heat feedback model is Karabeyoglu's model dependent on total mass flux. Combustion model is global single step reaction model for 4 chemical species or chemical equilibrium model for 9 chemical species. As a first step, steady-state solutions are reported.

Key Words: Hybrid Rocket, CFD, Thermal Conduction, Performance Prediction

Nomenclature

\begin{align*}
t & : \text{time} \\
x & : \text{axial location} \\
x_c & : \text{axial location at the chamber end} \\
x_e & : \text{axial location at the nozzle exit} \\
y & : \text{location normal to the solid fuel surface} \\
L & : \text{port length} \\
D_p & : \text{diameter of the port} \\
A & : \text{cross-sectional area} \\
l_p & : \text{perimeter of a cross-section} \\
\rho & : \text{density} \\
p & : \text{pressure} \\
T & : \text{temperature} \\
T_0 & : \text{base temperature} \\
u & : \text{x-direction velocity} \\
v & : \text{y-direction velocity} \\
G & : \text{total mass flux} \\
e & : \text{specific total energy} \\
e & : \text{specific internal energy} \\
h_i & : \text{specific enthalpy of chemical species } i \\
\Delta h_i^0 & : \text{standard enthalpy of formation of chemical species } i \\
c_{p,i} & : \text{specific heat of chemical species } i \text{ at constant pressure} \\
b_C & : \text{mole number of element C per unit mass of mixture gas} \\
\xi & : \text{mixture fraction} \\
\xi_\text{St} & : \text{stoichiometric mixture fraction} \\
Y_i & : \text{mass fraction of chemical species } i \\
r & : \text{regression rate} \\
m_f & : \text{mass addition from the solid fuel surface} \\
h_w & : \text{enthalpy of the fuel gas evaporating from the surface} \\
h_i & : \text{effective heat of gasification of the solid fuel} \\
Q_c & : \text{heat of combustion per unit mass of mixture gas} \\
w_i & : \text{molecular weight of chemical species } i \\
\mu & : \text{viscosity} \\
\lambda & : \text{thermal conductivity} \\
\alpha & : \text{thermal diffusivity} \\
R^0 & : \text{universal gas constant} \\
B_T & : \text{thermochemical blowing parameter} \\
B_a & : \text{aerodynamic blowing parameter} \\
C_f/C_{f0} & : \text{ratio of skin-friction coefficient with/without surface blowing} \\
q, k & : \text{constant parameters in Eqs. (12), (21)} \\
A_0 & : \text{preexponential factor} \\
E_a & : \text{activation energy} \\
a, n & : \text{constant parameters in Eq. (22)} \\
a', m & : \text{constant parameters in Eq. (25)} \\
\end{align*}

Subscripts

\begin{align*}
1 & : \text{fuel stream} \\
2 & : \text{oxidizer stream} \\
r & : \text{reference} \\
s & : \text{solid} \\
g & : \text{gas} \\
a & : \text{ambient} \\
S & : \text{solid fuel surface} \\
f & : \text{flame location} \\
e & : \text{boundary layer edge} \\
F & : \text{fuel} \\
O & : \text{oxidizer} \\
\end{align*}
Hybrid rocket propulsion is considered to be promising technology for the next generation space transportation. In a typical hybrid rocket, the fuel is solid and the oxidizer is liquid or gas. Merits of a hybrid rocket are high safety and high theoretical specific impulse compared to those of a solid rocket, and so on. On the other hand, there are some technical challenges to be overcome before putting a hybrid rocket into practical use; such as slow regression rate, low efficiency of combustion and combustion instability. The mechanism characterizing hybrid rocket is boundary layer combustion. In this mechanism, various phenomena interact intricately. For example, fluid phenomena in main stream, thermal conduction into the solid fuel, fuel gasification and liquefaction, chemical reaction, etc. A schematic of boundary layer combustion is shown in Fig. 1.

Previous studies about numerical simulations of hybrid rocket internal ballistics are, for example, the analysis of combustion instability by Stoia-Djeska et al., Politehnica University of Bucharest\(^1\), and the simulations of fuel regression by Antoniou et al., University of New Orleans\(^2\). However, overall analysis over a burning time is not conducted enough.

The final purpose of this study is to develop a design tool for prediction of hybrid rocket performance, such as regression rate characteristics and combustion stability, from ignition time to end of combustion. When internal phenomena in a hybrid rocket chamber are described, it is difficult to use rigorous models for this target. It is because calculation cost may be too expensive. Therefore simple models are required for this calculation. In this study, fluid phenomenon of main stream and thermal conduction phenomenon in a solid fuel are considered, because characteristic times of these phenomena are longer than those of other phenomena. Hence, these phenomena are coupled and solved. On the other hand, characteristic times of combustion reactions are short enough, and quasi-steady flame is assumed. The energy balance equation at the solid fuel surface is solved to estimate regression rate. In order to examine the effectiveness of the method using these models, as a first step, steady state analysis is done by the method.

2. Method

2.1. Configuration

Calculation domain is in a hybrid rocket chamber and a nozzle. A fuel grain has a circular single port. Configuration of the port and the nozzle is shown at Fig. 2 and Table 1. Variation of the port diameter through time is not considered for the moment.

![Configuration of a hybrid rocket chamber.](image)

<table>
<thead>
<tr>
<th>Variable [Unit]</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length of the port [cm]</td>
<td>60.0</td>
</tr>
<tr>
<td>Diameter of the port [cm]</td>
<td>4.00</td>
</tr>
<tr>
<td>Diameter of the nozzle throat [cm]</td>
<td>1.79</td>
</tr>
</tbody>
</table>

Fuel is polyethylene. Oxidizer is oxygen. It is assumed that any polyethylene becomes ethylene when the solid fuel gasifies and that liquid oxygen has already evaporated when it is injected into the chamber.

2.2. Basic equations for flowfield

Basic equations for flowfield are the quasi-one-dimensional compressible Euler equations with a conservation equation for the mixture fraction. Mass addition from the solid fuel surface is considered as a source term.

\[
\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = S_{QID} + S_{mass} \tag{1}
\]

\[
Q = \begin{bmatrix} \rho \\ \rho u \\ \rho e_t \\ \rho \xi \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p) \xi \\ \rho \xi \end{bmatrix},
\]

\[
S_{QID} = \begin{bmatrix} 0 & -\rho dA & 0 & 0 \\ p dA & 0 & 0 & 0 \\ 0 & 0 & l_p \dot{m}_F & 0 \\ 0 & 0 & l_p \dot{m}_F \end{bmatrix}, \quad S_{mass} = \begin{bmatrix} 0 \\ 0 & l_p \dot{m}_F \end{bmatrix}
\]

These equations are solved numerically. Boundary conditions at head end of the chamber are subsonic inflow conditions as
2.3. Thermal conduction into the solid fuel

Heat balance at the solid fuel surface is expressed by Eq. (7). Radiation heat transfer is not considered for the moment.

\[
\lambda_s \left( \frac{\partial T}{\partial y} \right)_{y=0} = \lambda_g \left( \frac{\partial T}{\partial y} \right)_{y=\infty} - \rho_f \dot{r} h_v
\]

(7)
y is the location normal to the solid fuel surface. The solid fuel surface is at \( y = 0 \). The inside of the solid fuel is at \( y < 0 \). It is assumed that the solid fuel is semi-infinite, i.e. \(-\infty < y \leq 0\). The left-hand side of this equation means the term of thermal conduction into the solid fuel. The first term in the right-hand side of this equation means heat feedback from the flame, while the second term means the energy required for the solid fuel to evaporate.

In the left-hand side of Eq. (7), temperature profile in the solid fuel is obtained by solving one-dimensional thermal conduction equation at any location \( x \).

\[
\frac{\partial T}{\partial t} + r \frac{\partial T}{\partial y} - \alpha_s \frac{\partial^2 T}{\partial y^2} = 0
\]

(8)

Boundary conditions follow.

\[
T = T_s \quad \text{at} \quad y = 0
\]

(9)

\[
T = T_a \quad \text{at} \quad y = -\infty
\]

(10)

In a steady state, analytical solution of this equation can be obtained.

\[
T(y) = T_s + \left( T_s - T_a \right) \exp \left( \frac{\dot{r}}{\alpha_s} y \right)
\]

(11)

First term in the right-hand side of Eq. (7) is evaluated by quasi-steady flame model, such as Karabeyoglu's model 16). Karabeyoglu's model is based on Marxman's turbulent boundary layer combustion model 17). While thermochemical blowing parameter is equal to aerodynamic blowing parameter in Marxman's model, Karabeyoglu distinguishes these parameters. Constant parameters \( a, k \) are the parameters related to blocking effect. The details of these parameters are described at section 2.5. Heat feedback behavior depends on mass flux in this model.

\[
\dot{r} = A_r \exp \left( - \frac{E_r}{R T_s} \right)
\]

(12)

Regression rate \( \dot{r} \) is eliminated from Eq. (7) by using this equation. Hence, Eq. (7) is expressed as the equation of temperature at the solid fuel surface \( T_s \). When this equation is solved for \( T_s \), \( \dot{r} \) and \( \dot{m}_f \) (\( = \rho f \dot{r} \)) are obtained.

2.4. Combustion model

Many chemical species take part in combustion reactions. And a lot of elementary processes make progress at the same time. When a calculation for combustion is done, it is difficult that all chemical species and all elementary processes are considered. Hence, the combustion model should deal with only significant chemical species and elementary processes over the combustion process. In this study, two combustion models are used. One model is global single step reaction model for 4 chemical species. The other model is chemical equilibrium model for 9 chemical species.

2.4.1. Global single step reaction model for 4 chemical species

It is assumed that characteristic time of chemical reaction is short enough and that fuel gas and oxidizer are mixed and reacted instantly in the control volume. Four chemical species \( \text{C}_2\text{H}_4, \text{O}_2, \text{CO}_2, \text{H}_2\text{O} \) are considered. Combustion reaction is assumed to be a global single step reaction.

\[
\text{C}_2\text{H}_4 + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O}
\]

(14)
Backward reaction of Eq. (14) is not considered. With those assumptions, mass fraction $Y$ is related to mixture fraction $\xi$ as Fig. 3.

2.4.2. Chemical equilibrium model for 9 chemical species

It is assumed again that fuel gas and oxidizer are mixed and reacted instantly in the control volume. With NASA CEA code\(^3\), chemical species are selected so that the flame temperature in limitation of chemical species is nearly equal to that in no limitation of chemical species. As the results, nine chemical species $C_2H_4$, $O_2$, $CO_2$, $H_2O$, $CO$, $H_2$, $OH$, $O$, $H$ are considered. Particular reaction processes are not considered. Temperature and chemical composition are obtained with chemical equilibrium calculation. In this calculation, free energy is minimized by Lagrange’s method of undetermined multipliers under the constraint condition that mole numbers of elements are conserved\(^7\). In the case of a constant-pressure change, Gibbs free energy is used for the free energy minimization, and the values of pressure and enthalpy are required. In the case of a constant-volume change, Helmholtz free energy is used for the free energy minimization, and the values of density and internal energy are required.

In this study, Helmholtz free energy minimization is employed. This method is easy to be combined with CFD calculation, because density and internal energy are the conservative quantities in the flowfield. And, this method does not need the iterative calculation (tentative determination of pressure, free energy minimization, re-determination of pressure) as required in Gibbs free energy minimization method. Maximum temperature obtained by this method is higher than that obtained by Gibbs free energy minimization method, because a constant-volume change is assumed in this method. Since pressure is nearly constant in a rocket chamber, Gibbs free energy minimization method is suitable for the calculation of the flowfield in the chamber. The reason why the Helmholtz free energy minimization method is employed is that the difference of maximum temperature is relatively small (the difference is estimated by thermodynamics approach within only 20% of the maximum temperature at a constant-pressure change). Hence, the easiness to be combined with CFD is accorded priority over the accuracy for the moment. This point will be improved by using Gibbs free energy minimization method.

2.5. Estimation of the parameters $\bar{B}$, $q$, $k$

Thermochemical blowing parameter $\bar{B}$ affects heat transfer in boundary layer. This parameter is defined as follows.

$$B_i = \frac{u_c}{u_f} \frac{h_{fl} - h_g}{h_f}$$ (15)

The specific enthalpy at the flame $h_{fl}$ and the specific enthalpy at the surface $h_g$ are defined with base temperature $T_0 = 298.15 \text{[K]}$. It is assumed that the gas composition at the wall is 100% fuel.

$$h_{fl} = h_f(T_f) - h_p(T_0)$$ (16)

$$h_g = h_f(T_S) - h_f(T_0)$$ (17)

When it is assumed that the process is adiabatic, the specific enthalpy at the flame is equal to the heat of combustion per unit mass of mixture gas $Q_f$.

$$h_{fl} = Q_c$$ (18)

$Q_c = 10900 \text{[kJ/kg]}$ is used in the 4 species case and $Q_c = 5300 \text{[kJ/kg]}$ is used in the 9 species case. Surface temperature $T_s \approx 880 \text{[K]}$ is used in order to estimate the specific enthalpy at the surface. These values are estimated with the results of our previous simulations\(^4\). Effective heat of gasification $h_t = 2700 \text{[kJ/kg]}$ is used\(^5\). For simplicity, it is assumed that boundary layer velocity profile does not vary along the axial direction and the velocity ratio $u_c/u_f$ is constant. In this study, the value estimated by Marxman et al. is used as the ratio, $u_c/u_f = 1.8$\(^\text{6}\). However, boundary layer velocity profile is not uniform along the axial direction\(^7\). This point will be improved in the next step. Considering the above values, $B_i$ is 6.1 in the 4 species case and $B_i$ is 2.7 in the 9 species case.

The ratio of skin-friction coefficient with/without surface blowing $C_f/C_{f0}$ means the reduction in skin-friction caused by surface blowing, which is called “blocking effect”. Marxman expressed the factor $C_f/C_{f0}$ as an experimental relation to aerodynamic blowing parameter $B_a$\(^9\).

$$\frac{C_f}{C_{f0}} = \left[ \frac{\ln(1 + B_a)}{B_a} \right]^{0.8} \left[ 1 + 1.3B_a + 0.364B_a^2 \right]^{0.2} \left( 1 + 0.5B_a \right)$$ (19)

$$B_a = \frac{(\rho y)_{inf}}{\rho \mu C_f/2} = \frac{\rho_f \dot{h}}{GC_f/2}$$ (20)

He also suggested the simplified expression in a particular range of $B_a$:

$$\frac{C_f}{C_{f0}} = qB_a^{-k}$$ (21)

The constant parameters $q$, $k$ in Eq. (12) are defined by this equation (21). In this study, the range $1 \leq B_a \leq 15$ is...
considered. When Eq. (19) is simplified in this range of $B_\alpha$, $q = 0.74$ and $k = 0.53$ are obtained.

### 2.6. Discretization

Basic equations for flowfield are discretized with finite volume method. Numerical flux is evaluated with AUSMDV scheme which is famous as a robust scheme. In order to achieve higher order accuracy for space, second-order MUSCL method is used. Time integration is two-stage Runge-Kutta method.

### 3. Results

#### 3.1. Temperature profile in the chamber

For the case that injection mass flux is 120 [kg/s/m$^2$], calculations are done and steady state solutions are obtained. Temperature profiles in the chamber are shown in Fig. 4. In the case with the model considering 4 chemical species, the maximum temperature is about 6000 K. With NASA CEA code on the condition of no limitation of chemical species, chamber temperature in the stoichiometric combustion of $\text{O}_2/\text{C}_2\text{H}_4$ is estimated as 3500 K. The maximum temperature is much higher than the temperature obtained by CEA. This is completely different from real phenomena. On the other hand, the maximum temperature is just over 3000 K in the case with the model considering 9 chemical species. This is relatively close to real phenomena. It is because, as shown in Fig. 5, combustion products are partially pyrolyzed to form CO and OH, etc.

![Fig. 4. Temperature profile in the chamber at steady state.](image)

#### 3.2. The effect of oxygen mass flux on regression rate

For five cases that $G_{inj} = 60, 120, 170, 230, 280$ [kg/s/m$^2$], calculations are done and steady state solutions are obtained. Regression rate profiles obtained as the results are averaged for the axial direction in each case. The graph of the relation between average regression rate and injection mass flux (oxygen mass flux) is shown in Fig. 6. The data of the literature is also shown in Fig. 6. The meanings of the signs in Fig. 6 are in Table 3. The average regression rate obtained with the model considering 4 chemical species is about 1.7 times as high as that obtained with the model considering 9 chemical species. The main cause follows as: (i) The flame temperature in the 4 chemical species case is higher than that in the 9 species case. (ii) The thermochemical blowing parameter [Eq. (15)] in the 4 species case is larger. (iii) The heat feedback from flame [Eq. (12)] in the 4 species case is higher. Hence, thermochemical blowing parameter $B_\alpha$ is very important for the prediction of regression rate.

![Fig. 5. Mass fraction profile in the chamber at steady state (in the case with the model considering 9 chemical species).](image)

![Fig. 6. The relation between average regression rate and injection mass flux (oxygen mass flux).](image)

![Table 3. The meanings of the signs in Fig. 6.](image)

<table>
<thead>
<tr>
<th>Sign</th>
<th>Injection type</th>
<th>Sign</th>
<th>Fuel type</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Axial-flow injection</td>
<td>1</td>
<td>Conventional fuel</td>
</tr>
<tr>
<td>B</td>
<td>Swirl injection</td>
<td>2</td>
<td>Aluminized fuel</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3</td>
<td>Cryogenic solid fuel</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>Paraffin-based fuel</td>
</tr>
</tbody>
</table>

Calculation results fit in Eq. (22).

$$\dot{r}_{ave} = aG_{inj}^n$$

The constant parameter $a$, $n$ are determined by least-square method.

$$\dot{r}_{ave} = 0.0168G_{inj}^{0.763} \quad (4 \text{ chemical species})$$

Pa_75
Scaling effect is evaluated with Eq. (25) 12). In these equations, the unit of \( \dot{r}_{ave} \) is [mm/s] and the unit of \( G_{inj} \) is [kg/s/m²]. Injection type of the rocket simulated in this study is A type; "Axial-flow injection". Fuel type of the rocket simulated is 1 type; "Conventional fuel". In Fig. 6, calculation results close to the A1 group of the literature's data. It is confirmed that the order of regression rate of the simulation is nearly equal to that of the literature.

3.3. The effect of port length on regression rate

At section 3.1 and section 3.2, the port length \( L \) is 0.60 [m]. In this section, for five cases that \( L = 0.20, 0.30, 0.60, 0.80, 1.3 \) [m], calculations are done and steady state solutions are obtained. Injection mass flux is 120 [kg/s/m²]. As a combustion model, the chemical equilibrium model for 9 chemical species is used. The ratio of port length and port diameter \( L/D_p \) and nozzle area ratio are constant in all cases. Scaling effect is evaluated with Eq. (25) 13):

\[
\dot{r}_{ave} = a' G_{inj}^{0.769} L_n^{\text{avg}} \quad \text{(25)}
\]

The constant parameter \( a', m \) are determined by least-square method. The parameter \( n \) is determined at section 3.2.

\[
\dot{r}_{ave} = 0.00875 G_{inj}^{0.769} L^{0.228} \quad \text{(26)}
\]

In this equation, the unit of \( \dot{r}_{ave} \) is [mm/s] and the unit of \( G_{inj} \) is [kg/s/m²]. And, the unit of \( L \) is [m]. The graph of the relation between average regression rate and port length is shown in Fig. 7. The average regression rate is proportional to \( L^{0.228} \).

Fig. 7. The relation between average regression rate and port length.

4. Conclusion

In this study, the coupling method of CFD and thermal conduction calculation was developed. Two combustion models were used in this method. One model was global single step reaction model for 4 chemical species. The other model was chemical equilibrium model for 9 chemical species. Steady state calculations were done with this method, and the usability of this method was examined.

- The global single step reaction model for 4 chemical species is not appropriate to predict the state in the chamber, because the maximum temperature is enormously high.
- The order of regression rate of the simulation is nearly equal to that of the literature.
- Thermochemical blowing parameter \( B_i \) is very important for the prediction of regression rate.
- Scaling effect was evaluated with the equation \( \dot{r}_{ave} = a' G_{inj}^{0.769} L_n^{\text{avg}} \).

As future works, the method will be modified. The calculation method of chemical equilibrium will be changed into Gibbs free energy minimization method. In order to estimate \( B_i \) with more precision, the axial change of the velocity ratio \( u_L/u_p \) will be considered. After the modifications, parametric studies will be done in order to examine hybrid rocket internal ballistics.

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References