Development of Wall Regression Model of Hybrid Rocket Solid Fuel

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The purpose of this study is to develop a computational method to predict fuel regressions for hybrid rocket solid fuels. The shape of the flow field changes depending on the regression and vaporization of the solid fuel. This shape change and the heat flux from the combustion gas to the fuel are mutually dependent. Therefore a computational method that can accurately predicts both of the fuel regression and the heat flux is necessary to clarify the mutual dependence of them. In this study, we have developed a computational method to predict the regression phenomenon including the effect of the shape change of the flow field. The developed code predicts the regression phenomena by repeating gas-phase calculations and regression-phase calculations. The wall consisting of grids permits the flow field to be an arbitrary shape. As the first step, the complex chemical reaction was not included and numerical results were compared with a sublimation phenomenon of naphthalene in a non-combustion flow. Numerical results successfully predicted Nusselt number change due to regression qualitatively.

**Key word:** Hybrid Rocket, CFD, Regression, Impinging jet

**Nomenclature**

\[
\begin{align*}
A_{ij} & : \text{heating area of cell} \\
C_p & : \text{specific heat at constant pressure} \\
d & : \text{nozzle width} \\
e & : \text{total energy} \\
h & : \text{heat transfer coefficient} \\
h_p & : \text{mass transfer coefficient} \\
H & : \text{initial nozzle – sample surface distance} \\
\Delta H & : \text{effective heat of gasification} \\
\Delta H_{ij} & : \text{effective heat of gasification of a cell} \\
k & : \text{turbulent kinetic energy} \\
Le & : \text{Lewis number} \\
\dot{m} & : \text{mass transfer rate} \\
Nu & : \text{Nusselt number} \\
n & : \text{time step} \\
P & : \text{static pressure} \\
P_w & : \text{saturated vapour pressure of naphthalene} \\
P_k & : \text{production rate of k} \\
P_r & : \text{Prandtl number} \\
\dot{Q} & : \text{heat transfer per unit area to the wall} \\
R & : \text{gas constant} \\
Re & : \text{Reynolds number} \\
\dot{S}_{ij} & : \text{strain rate} \\
Sc & : \text{Schmidt number} \\
t & : \text{time}
\end{align*}
\]

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1. Introduction

Hybrid rockets have the advantage of enhanced safety from explosion or detonation during fabrication, storage, and operation. This advantage is feasible to produce frequent private-sector commercial missions or potentially less-expensive sounding rockets. However, hybrid rockets have a serious problem of low thrust as a result of low gasification rates, which are typically less than one-third those of composite solid rocket propellants. To resolve this problem, several new ideas have been proposed and/or developed, such as a swirling-oxidizer-type or cascaded multi-stage impinging-jet (CAMUI) type.\(^{1,3}\)

In a combustion chamber of a hybrid rocket engine, the channel wall surrounding the combustion field is a solid fuel. The shape of the flow field changes depending on the regression and vaporization of the solid fuel. In a CAMUI-type fuel grain, there are multiple types of burning surfaces. Because the regression progress is complicated, predicting the regression progress and vaporization of the solid fuel is necessary to clarify the mutual dependence between them. Therefore a computational method that can accurately predict both of the fuel regression and the heat flux is required.

When the solid fuel regresses, the flow channel geometry changes simultaneously. This geometry change and the heat flux from the combustion gas to the fuel are mutually dependent. Therefore a computational method that can accurately predict both of the fuel regression and the heat flux is necessary to clarify the mutual dependence between them. In this study, the authors have developed a computational method to predict the regression phenomenon including the effect of the shape change of the flow channel. This algorithm comes from the one developed by Suzuki et al. to predict sand erosion phenomenon.\(^{5,6}\) To verify the validity of the model, naphthalene sublimation experiments were conducted.

2. Numerical Procedures

2.1. Assumption

Because the time scales of flow and the wall regression are in a different order of magnitude with each other, the model assumes a quasi-steady process for the shape change of the flow field. The computational procedure for the prediction of the wall regression is as follows:

1. Calculate the flow field.
2. Calculate the heat flux from the gas to the wall.
3. Estimate the amount of regression.
4. Change the wall shape.
5. Return to [1].

This procedure is repeated iteratively, until the computational time reaches the prescribed terminal time.

2.2. Flow field calculation

In the present work, we used a numerical simulation code based on a finite difference method. Time averaged compressible Navier-Stokes equations were solved until it reaches a steady state. The governing equations with the \(k - \varepsilon\) model are expressed as follows:

Continuity equation
\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0
\]  
(1)

Navier-Stokes equation
\[
\frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) =
\frac{\partial}{\partial x_j} \left\{ \left( \mu + \frac{\mu}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} - \frac{2}{3} \rho \varepsilon \frac{\partial u_i}{\partial x_j} \right\}
\]  
(2)

Energy equation
\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_j} (\rho e u_j) =
\frac{\partial}{\partial x_j} \left\{ \left( \mu + \frac{\mu}{\sigma_k} \right) \frac{\partial e}{\partial x_j} \right\} + \rho (P_i - \varepsilon)
\]  
(3)

\(k - \varepsilon\) model
\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left\{ \left( \mu + \frac{\mu}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} \right\}
+ \rho \frac{\varepsilon}{k} (C_{nu} P_i - C_{nu_e} \varepsilon)
\]  
(5)

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left\{ \left( \mu + \frac{\mu}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} \right\}
+ \rho \frac{\varepsilon}{k} (C_{nu} P_i - C_{nu_e} \varepsilon)
\]  
(6)

\(k\) and \(\varepsilon\) are turbulent kinetic energy and its dissipation rate, respectively. Since the standard \(k - \varepsilon\) model excessively predicts turbulent energy production for irrotational strain, Kato-Lauder’s modification was adopted.

\[/eq]
\[
\frac{\partial}{\partial t} \tilde{S} + \frac{\partial}{\partial x_j} (\tilde{S} u_j) = \frac{1}{2} \frac{\partial}{\partial x_j} \left( \tilde{S} \frac{\partial \tilde{S}}{\partial x_j} \right) \]
\[
\tilde{S} = \frac{1}{2} \frac{1}{2} (S_u S_\tilde{S} + S_\tilde{S} S_u), \tilde{\Omega} = \frac{1}{2} \Omega_u \Omega_y
\]  
(8)

where \(C_{nu} = 0.09, \sigma_k = 1.0, \sigma_\epsilon = 1.3, C_{nu_e} = 1.44, \tilde{C}_{nu_2} = 1.92.\)
A convection term in the momentum equation is discretized by 2nd order upwind TVD scheme. A viscous term is estimated by the 2nd order central scheme. The 4-stage Runge-Kutta method was applied to the time integration.

2.3. Wall regression estimation

The formulation of a hybrid combustion theory requires consideration of the process of heat transfer from the flame to the wall. The regression rate \( r \) is given by

\[
\dot{r} = \frac{Q}{\Delta H}.
\]

In the computational model, walls consist of grids. Therefore the computation grid consists of the wall region and the flow filed region. Changing a wall cell to a flow field cell permits the flow field to be an arbitrary shape (Fig. 1). The effective heat of gasification of a cell \( \Delta H_{ij} \) can be expressed as follow:

\[
\Delta H_{ij} = \rho_{ij} V_{ij} \Delta H
\]

The accumulation of heat input from the flow field to a wall cell is defined as \( \eta_{ij} \). Temporal progress of \( \eta_{ij} \) \((n \rightarrow n + 1)\) is expressed as follows:

\[
\eta_{ij}^{n+1} = \eta_{ij}^n + \frac{Q_{ij}^n \Delta t}{\Delta H_{ij}}.
\]

When a wall cell satisfies the following condition, the wall cell changes to a flow field cell.

\[
\eta_{ij}^{n+1} \geq \Delta H_{ij}
\]

Surplus heat input is took over as \( \eta_{ij}^{n+1} \) by the underlying cell.

The local mass transfer rate \( m \) at any surface location can be evaluated from the local change of surface elevation. The mass transfer coefficient \( h_{ij} \) is expressed as follow:

\[
h_{ij} = \frac{m}{\rho_{w} - \rho_{\infty}} = \frac{RT_{w} \rho_{s} \delta}{p_{v} t_{f}}
\]

where \( \rho_{w} \) is wall naphthalene vapour density, \( \rho_{\infty} \) is naphthalene vapour density in main stream \((\rho_{\infty} = 0)\), \( R_{g} \) is gas constant of naphthalene, \( p_{v} \) is saturated vapour pressure of naphthalene and \( \rho_{s} \) is the density of solid naphthalene.

According to the analogy, the conversion between the mass transfer and heat transfer coefficients at the same Reynolds number can be accomplished by the following relation.

\[
\frac{h_{ij}}{h_{ij}} = 4.0 \left( \frac{Pr}{Sc} \right)^{0.4}.
\]

Therefore heat transfer coefficients are obtained from experiment results by

\[
h = h_{ij} \left( \frac{Sc}{Pr} \right)^{0.6}.
\]

Since the experiments were conducted at room temperature, the Prandtl number is 0.71 for air and the Schmidt number is 2.28 for the naphthalene vapour.

The heat transfer coefficient of numerical results is defined by

\[
h = \frac{Q}{T_{w} - T_{\infty}}.
\]

Nusselt number \( Nu\) is defined as

\[
Nu = \frac{h \lambda}{\lambda}
\]
3.2. Apparatus

Experiments were conducted using naphthalene and air. The naphthalene samples were casted using silicone mold. Table 1 shows the properties of the naphthalene samples. The density of a naphthalene sample was determined by weighing the sample by a digital weight gauge.

Table 1. Naphthalene properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight of gas</td>
<td>128.2[g/mol]</td>
</tr>
<tr>
<td>Density of solid of naphthalene, $\rho_s$</td>
<td>1.01[g/cm³]</td>
</tr>
<tr>
<td>Latent heat of sublimation</td>
<td>133[kcal/kg]</td>
</tr>
<tr>
<td>Gas constant, $R_s$</td>
<td>6.62[J/kg K]</td>
</tr>
<tr>
<td>Saturated vapour pressure of naphthalene, $P_{v,w}$</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature [°C]</th>
<th>$P_{v,w}$ [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.8</td>
</tr>
<tr>
<td>5</td>
<td>1.33</td>
</tr>
<tr>
<td>10</td>
<td>2.80</td>
</tr>
<tr>
<td>15</td>
<td>4.67</td>
</tr>
</tbody>
</table>

Figure 2 shows a cut way diagram of the experimental domain. Air was supplied from a compressor and a needle valve and a flow meter regulate the flow rate. The naphthalene sample was placed on a stainless steel base and held in place by sandwiching the sides with fixtures, stainless steel wall, and a glass window. Air was fed from a slit nozzle above the sample. The flat air flow creates a quasi-two dimensional flow field, which is uniform along the depth direction of the figure.

Table 2. Nozzle properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle width, $d$</td>
<td>2 [mm]</td>
</tr>
<tr>
<td>Nozzle – wall distance, $H$</td>
<td>4 [mm]</td>
</tr>
<tr>
<td>Nozzle depth</td>
<td>20 [mm]</td>
</tr>
<tr>
<td>Sample width</td>
<td>34 [mm]</td>
</tr>
<tr>
<td>Sample height</td>
<td>19 [mm]</td>
</tr>
<tr>
<td>Sample depth</td>
<td>20 [mm]</td>
</tr>
</tbody>
</table>

4. Computational Conditions

Figure 4 shows the boundary conditions. To correspond to the mass transfer experiment, the boundary conditions were imposed as follows. At the inlet boundary, mass flow rate and temperature were fixed. The mass flow rate is same value as experimental value. Therefore the Reynolds number of numerical condition corresponds to the Reynolds number of experimental condition. The mass flow rate was determined by considering sublimation speed of naphthalene. At the exit, static pressure was specified. On the upper wall, non-slip and adiabatic conditions were imposed. The adiabatic condition of upper wall corresponds to conditions of no mass transfer of experiment. On the sample wall surface, non-slip and isothermal conditions were used. Table 3 shows the calculation conditions. We consistently used a structured mesh. The computational grid consists of two regions, a flow field and a solid wall. The cell height in the wall is uniform and the same as the minimum one in the flow field. Figure 4 shows the computational grids. The total grid number is 48,000.

Table 3. Calculation conditions.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate</td>
<td>24.5 [kg/m² S]</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>293 [K]</td>
</tr>
<tr>
<td>Sample wall temperature</td>
<td>313 [K]</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>101 [kPa]</td>
</tr>
</tbody>
</table>

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Pa_70
5. Results and Discussion

5.1. Change of flow field

Figure 5 shows the change of the flow filed due to regression. The shape of the flow field changes as a result of the regression.

Significant regression occurs in the impingement region. It is known that, when jet strikes a wall surface, it forms an extremely thin stagnation boundary layer which offers little resistance to heat flow. The numerical result reproduces the phenomenon. Figure 6 shows the lateral distribution of normalized vertical velocity at normalized distance 0.5 from the wall surface. The velocity is normalized by the average velocity of the inlet \( u_{in} \). The red and blue lines show the normalized velocity before and after regression, respectively. The air stream velocity decreases with the progress of the regression. This decrease is due to the interference between the main stream and the wall jet.

Figure 7 shows comparison of the stagnation Nusselt number. The horizontal axis is normalized surface regression depth at the stagnation point, and the vertical axis is the stagnation Nusselt number. The blue and black circles show numerical and experimental results, respectively. The blue circles show numerical results supposing uniform regression, i.e., only the nozzle-wall distance increases without any change of the wall shape. The numerical and experimental results show the same trend. On the other hand, the stagnation Nusselt number is independent on the regression depth for the case supposing uniform regression. In the numerical result, the stagnation Nusselt number decreases as the regression depth increases. This trend agrees with the experimental trend. It is known that the increase of the ratio of the nozzle-wall distance to nozzle width \( H / d \) reduces the stagnation Nusselt number. However, in the potential core region \( (H / d \leq 4) \), the stagnation Nusselt number is independent on the ratio because it depends only on the Reynolds and Prandtl numbers. After regression, the maximum value of the ratio was less than 4, meaning that it is still in the potential core region. The decrease in the stagnation Nusselt number is due to the curvature of the wall surface. As the regression proceeds, the curvature of wall surface develops. A past study has revealed that Nusselt number decreases as a result of the curvature developed in the stagnation region. In the present study, the trends of Nusselt number agree with the previous study.
5.2. Regression distribution

Figure 8 shows the distribution of the regression depth. The red squares show the experiment result. The blue circles show numerical results assuming that the heat input is through only the upper surface of each cell. The black circles show numerical results assuming that the side surface of each cell contributes as a thermal flow path. These two different assumptions do not cause a large difference. Although the quantitative agreement is limited, the numerical results qualitatively replicate the experiment result. The deviations are mainly due to the deficient predictability of the temperature gradient near the wall.

6. Conclusion

The purpose of this study is to develop a computational method to predict fuel regression for hybrid rocket solid fuels. The authors have developed a computational method to predict the regression phenomenon including the effect of the shape change of the flow channel. To verify the validity of the model, naphthalene sublimation experiments were conducted. Regression distributions of the naphthalene sample were compared with numerical results. The developed code reproduces the regression phenomena by repeating gas-phase calculations and regression-phase calculations. The numerical result successfully predicted the Nusselt number change due to regression qualitatively. The distributions of regression depth were predicted qualitatively.

References