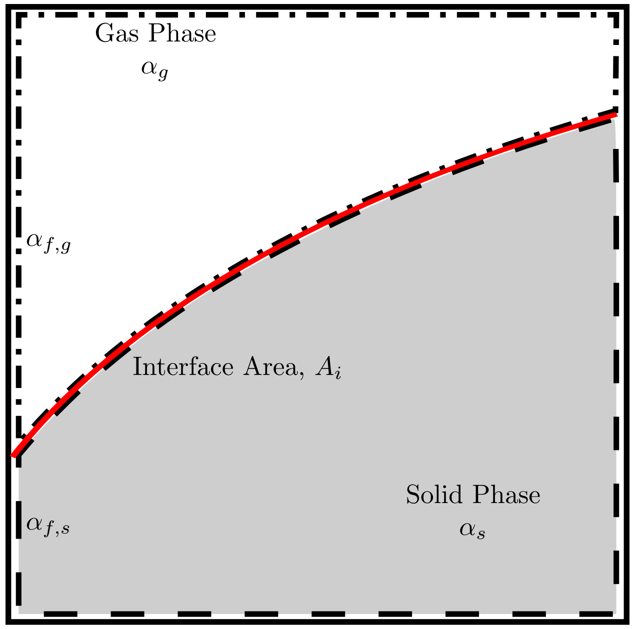

Figure 1: Diagram of Interface Cell

1 Governing Equations

The governing equations for the gas and solid portion of a given cell are derived in the following section. Figure 1 shows a representative cell within the domain that contains a volume fraction of solid and gas denoted by α_s and α_g respectively. Each cell face is also assigned a solid and gas face fraction (α_f) based on the amount of face area that is covered by the solid and gas. Finally, the interface area (A_i) represents the boundary between the solid and gas domains within the cell. The decomposition of each cell and determination of the volume fractions, face fractions, and interface area will be covered in Section **??**.

1.1 Solid Phase

The mass continuity equation for the shaded solid control volume is

$$\frac{\partial}{\partial t}\int_{V_s}\rho_s \mathrm{d}V_s + \int_{A_s}\rho_s(\hat{u}_{rel}\cdot\hat{n})\mathrm{d}A_s = 0.$$

Discretizing the solid continuity equation using a first-order approximation in time and a second-order approximation for the surface integral, the equation is written as

$$\frac{\rho_s V_s - \rho_s^0 V_s^0}{\Delta t} + \sum_{f,s}\rho_s(\hat{u}_{rel}\cdot\hat{A}_{f,s}) = 0.$$

Assuming that the solid is incompressible, the surface is regressing at a constant rate ($\dot{r}$), and the solid phase is stationary, the continuity equation becomes

$$\frac{V_s - V_s^0}{\Delta t} = -\frac{\dot{m}'' A_i}{\rho_s},$$

where $\dot{m}'' = \rho_s\dot{r}$. Furthermore, transferring the equation from the solid control volume to the cell control volume using the volume and area fractions, the final form of the solid continuity equation is

$$\boxed{\frac{\alpha_s - \alpha_s^0}{\Delta t} = -\frac{\dot{m}'' A_i}{\rho_s V_c}.} \tag{1}$$

Similarly, the energy equation for the shaded solid control volume is

$$\frac{\partial}{\partial t}\int_{V_s}\rho_s c_s T_s \mathrm{d}V_s + \int_{A_s} c_s T_s(\rho_s \hat{u}_{rel}\cdot\hat{n})\mathrm{d}A_s - \int_{A_s}\rho_s c_s(\nabla T_s\cdot\hat{n})\mathrm{d}A_s = \int_{V_s} S_{T_s}\mathrm{d}V_s,$$

where S_{T_s} is any volumetric source within the solid domain. Discretizing the solid energy equation and assuming constant thermophysical properties within the solid yields

$$\rho_s c_s \frac{T_s V_s - T_s^0 V_s^0}{\Delta t} - \sum_f \rho_s c_s(\nabla T_s\cdot\hat{A}_{f,s}) = S_{T_s}V_s - \dot{m}'' c_s(T_i - T_{ref})A_i,$$

where T_i is the temperature of the solid at the interface and T_{ref} is a combustion reference temperature. Finally, transferring the equation from the solid volume to the entire cell volume shows that

$$\rho_s c_s \frac{T_s\alpha_s - T_s^0\alpha_s^0}{\Delta t} - \frac{1}{V_c}\sum_{f,s}\rho_s c_s(\nabla T_s\cdot\hat{A}_f\alpha_{f,s}) = S_{T_s}\alpha_s - \frac{\dot{m}'' c_s(T_i - T_{ref})A_i}{V_c}.$$

Using (1) in conjunction with

$$\frac{T_s\alpha_s - T_s^0\alpha_s^0}{\Delta t} = \alpha_s\frac{T_s - T_s^0}{\Delta t} + T_s^0\frac{\alpha_s - \alpha_s^0}{\Delta t},$$

the final form of the solid energy equation is obtained as

$$\boxed{\rho_s c_s\alpha_s \frac{T_s - T_s^0}{\Delta t} - \frac{1}{V_c}\sum_{f,s}\rho_s c_s(\nabla T_s\cdot\hat{A}_f\alpha_{f,s}) = S_{T_s}\alpha_s - \frac{\dot{m}'' c_s(T_i - T_s^0)A_i}{V_c}.} \tag{2}$$

1.2 Gas Continuity Equation

Mass continuity on gray (gas) control volume (Vg) surround by boundary Ag

$$\frac{\partial}{\partial t}\int_{V_g}\rho \mathrm{d}V_g + \int_{A_g}\rho(\hat{u}\cdot\hat{n})\mathrm{d}A_g = 0$$

Using second-order approximations of the integrals and a first-order time derivative

$$\frac{\rho V_g - \rho^0 V_g^0}{\Delta t} + \sum_{f,g}\rho(\hat{u}\cdot\hat{A_{f,g}}) = 0$$

Translate this to the full cell

$$V_c\frac{\rho\alpha_g - \rho^0\alpha_g^0}{\Delta t} + \sum_f \rho(\hat{u}\cdot\hat{A}_f)\alpha_f = \dot{m}'' A_i$$

Divide by cell volume, V_c, to give the equation in OpenFOAM form that we want to solve

$$\boxed{\frac{\rho\alpha_g - \rho^0\alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_f \rho(\hat{u}\cdot\hat{A}_f)\alpha_f = \frac{\dot{m}'' A_i}{V_c}} \tag{3}$$

1.3 Gas Momentum Equation

Conservation of momentum on gray (gas) control volume (Vg) surround by boundary Ag

$$\frac{\partial}{\partial t}\int_{V_g}\rho\hat{u}\mathrm{d}V_g + \int_{A_g}\hat{u}(\rho\hat{u}\cdot\hat{n})\mathrm{d}A_g + \hat{F}_p = \int_{V_g} S_{\hat{u}}\mathrm{d}V_g$$

Using second-order approximations of the integrals and a first-order time derivative

$$\frac{\rho\hat{u}V_g - \rho^0\hat{u}^0V_g^0}{\Delta t} + \sum_{f,g}\hat{u}(\rho\hat{u}\cdot\hat{A_{f,g}}) + \hat{F}_p = S_{\hat{u}}V_g$$

Translate this to the full cell

$$V_c\frac{\rho\hat{u}\alpha_g - \rho^0\hat{u}^0\alpha_g^0}{\Delta t} + \sum_{f}\hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \hat{F}_p\alpha_f = S(\hat{u})\alpha_gV_c + \hat{u_s}\dot{m}''A_i$$

It is important to note that the velocity of the solid is zero by definition and therefore does not add any additional momentum to the system. Divide by cell volume, V_c, to give the equation in OpenFOAM form that we want to solve

$$\boxed{\frac{\rho\hat{u}\alpha_g - \rho^0\hat{u}^0\alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_{f}\hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \frac{\hat{F}_p\alpha_f}{V_c} = S_{\hat{u}}\alpha_g} \tag{4}$$

1.4 Gas Energy Equation

Conservation of energy on the gray (gas) control volume surrounded by boundary Ag

$$\frac{\partial}{\partial t}\int_{V_g}\rho E\mathrm{d}V_g + \int_{A_g}(E+\frac{p}{\rho})(\rho\hat{u}\cdot\hat{n})\mathrm{d}A_g = \int_{V_g}S_E\mathrm{d}V_g$$

The total energy of the fluid can be rewritten in terms of the specific enthalpy (h_s) such that

$$\begin{aligned} K =& \frac{u^2+v^2+w^2}{2} \\ i =& h_s - \frac{p}{\rho} \\ E =& i + K \\ E =& h_s + K - \frac{p}{\rho} \end{aligned}$$

Substituting into the energy equation then yields

$$\frac{\partial}{\partial t}\int_{V_g}\rho(h_s + K - \frac{p}{\rho})\mathrm{d}V_g + \int_{A_g}(h_s+K)(\rho\hat{u}\cdot\hat{n})\mathrm{d}A_g = \int_{V_g}S_E\mathrm{d}V_g$$

Using second-order approximations of the integrals and a first-order time derivative

$$\begin{aligned} &\frac{\rho h_sV_g - \rho^0h_s^0V_g^0}{\Delta t} + \sum_{f,g}h_s(\rho\hat{u}\cdot\hat{A}_{f,g}) \\ +&\frac{\rho KV_g - \rho^0K^0V_g^0}{\Delta t} + \sum_{f,g}K(\rho\hat{u}\cdot\hat{A}_{f,g}) \\ +&\frac{pV_g - p^0V_g^0}{\Delta t} \\ =&S_EV_g \end{aligned}$$

Translate equation to full cell

$$
\begin{aligned}
&V_c\frac{\rho h_s\alpha_g-\rho^0h_s^0\alpha_g^0}{\Delta t}+\sum_f h_s(\rho\hat{u}\cdot\hat{A}_f)\alpha_f\\
+&V_c\frac{\rho K\alpha_g-\rho^0K^0\alpha_g^0}{\Delta t}+\sum_f K(\rho\hat{u}\cdot\hat{A}_f)\alpha_f\\
+&V_c\frac{p\alpha_g-p^0\alpha_g^0}{\Delta t}\\
=&S_E\alpha_g V_c
\end{aligned}
$$

Similar to the momentum equation, the solid does not contribute any kinetic energy to the flow due to it having zero velocity. Divide by cell volume, V_c, to give the equation in OpenFOAM form that we want to solve

$$
\boxed{
\begin{aligned}
&\frac{\rho h_s\alpha_g-\rho^0h_s^0\alpha_g^0}{\Delta t}+\frac{1}{V_c}\sum_f h_s(\rho\hat{u}\cdot\hat{A}_f)\alpha_f\\
+&\frac{\rho K\alpha_g-\rho^0K^0\alpha_g^0}{\Delta t}+\frac{1}{V_c}\sum_f K(\rho\hat{u}\cdot\hat{A}_f)\alpha_f\\
+&\frac{p\alpha_g-p^0\alpha_g^0}{\Delta t}\\
=&S_E\alpha_g
\end{aligned}
} \tag{5}
$$

1.5 Gas Species Equation

Conservation of a given species mass fraction (Y_i) on gray (gas) control volume (Vg) surround by boundary Ag

$$
\frac{\partial}{\partial t}\int_{V_g}\rho Y_i \mathrm{d}V_g+\int_{A_g}Y_i(\rho\hat{u}\cdot\hat{n})\mathrm{d}A_g+\int_{A_g}(\hat{G}_i\cdot\hat{n})\mathrm{d}A_g=\int_{V_g}S_{Y_i}\mathrm{d}V_g
$$

Using second-order approximations of the integrals and a first-order time derivative

$$
\frac{\rho Y_iV_g-\rho^0Y_i^0V_g^0}{\Delta t}+\sum_{f,g}Y_i(\rho\hat{u}\cdot\hat{A_{f,g}})+\sum_{f,g}(\hat{G}_i\cdot\hat{A_{f,g}})=S_{Y_i}V_g
$$

Translate this to the full cell

$$
V_c\frac{\rho Y_i\alpha_g-\rho^0Y_i^0\alpha_g^0}{\Delta t}+\sum_f Y_i(\rho\hat{u}\cdot\hat{A}_f)\alpha_f+\sum_{f,g}(\hat{G}_i\cdot\hat{A}_f)\alpha_f=S_{Y_i}\alpha_gV_c+Y_{i,b}\dot{m}''A_i
$$

Divide by cell volume, V_c, to give the equation in OpenFOAM form that we want to solve

$$
\boxed{
\begin{aligned}
&\frac{\rho Y_i\alpha_g-\rho^0Y_i^0\alpha_g^0}{\Delta t}+\frac{1}{V_c}\sum_f Y_i(\rho\hat{u}\cdot\hat{A}_f)\alpha_f\\
+&\frac{1}{V_c}\sum_{f,g}(\hat{G}_i\cdot\hat{A}_f)\alpha_f=S_{Y_i}\alpha_g+\frac{Y_{i,b}\dot{m}''A_i}{V_c}
\end{aligned}
} \tag{6}
$$

2 Interface Temperature and Phase Linking

The governing equations derived in Section 1 account for the transfer of mass, momentum, and species between the solid and gas phase; however, these governing equations only account for the energy transfer

Figure 2: Interface Transfer Diagram

between the domains due to the mass transfer and do not account for the energy conduction across the boundary or any surface fluxes that may be present such as the pyrolysis energy release.

Completing an energy balance across the infinitesimal solid gas interface leads to the equation

$$\dot{m}'' h_{s,s}[T_i] - k_s \frac{\partial T_s}{\partial x} + q''_{ext} - \dot{m}'' h_{s,g}[T_i] + k_g \frac{\partial T_g}{\partial x} = 0.$$

Applying a first order discretization to the derivatives and collecting similar terms, the equation is then rewritten as

$$\dot{m}''(h_{s,s}[T_i] - h_{s,g}[T_i]) - k_s \frac{T_i - T_s}{L_s} + k_g \frac{T_g - T_i}{L_g} + q''_{ext} = 0.$$

The first term in this equation contains the condensed phase heat release value, $Q_c = h_{s,s}[T] - h_{s,g}[T]$. Substituting this value into the equation and solving for the interface temperature yields

$$T_i = \frac{\dot{m}'' Q_c + k_s T_s / L_s + k_g T_g / L_g + q''_{ext}}{k_s / L_s + k_g / L_g} \tag{7}$$

Using this interface temperature, source terms for the solid and gas phase energy equation are determined. One method of applying consistent boundary conditions across the phase linking is to allow one boundary to have a constant temperature condition while the other boundary has a constant flux condition. The present code implements this method by setting a constant temperature boundary on the solid and a constant flux boundary on the gas. The additional solid source terms are

$$Sp_{t,s} = \frac{k_s A_i}{L_s V_c}$$
$$Su_{t,s} = \frac{k_s T_i A_i}{L_s V_c}$$

and the additional gas source terms are

$$Su_{t,g} = \frac{k_g (T_i - T_g) A_i}{L_g V_c}.$$

The addition of the above source terms lead to the following modified versions of the solid and gas governing equations respectively:

$$\boxed{\rho_s c_s \alpha_s \frac{T_s - T_s^0}{\Delta t} - \frac{1}{V_c} \sum_{f,s} \rho_s c_s (\nabla T_s \cdot \hat{A}_f \alpha_{f,s}) = S_{T_s} \alpha_s - \frac{\dot{m}'' c_s (T_i - T_s^0) A_i}{V_c} + Su_{t,s} - Sp_{t,s} T_s} \tag{8}$$

$$\boxed{\begin{aligned} &\frac{\rho h_s \alpha_g - \rho^0 h_s^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f h_s (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\ +&\frac{\rho K \alpha_g - \rho^0 K^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f K (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\ +&\frac{p \alpha_g - p^0 \alpha_g^0}{\Delta t} \\ =&S_E \alpha_g + \frac{\hat{q}_b \cdot \hat{A}_b}{V_c} + Su_{t,g}. \end{aligned}} \tag{9}$$

3 Small Cell Handling

A common problem in immersed boundary methods is that small cells within the domain cause numeric instability. Typically these small cells are solved using an approximation in order to limit the effect of the aforementioned instability. The approximation chosen in the current code is to determine the small cell values based on a steady state solution between the small cell and it's neighboring cells. The following section details the derivation of the small cell approximation for each governing equation.

3.1 Solid Energy Equation

Starting with the previously derived solid energy equation, 8, and removing the time varying terms, we end with the equation

$$-\frac{1}{V_c}\sum_{f,s}\rho_s c_s(\nabla T_s \cdot \hat{A}_f \alpha_{f,s}) = S_{T_s}\alpha_s - \frac{\dot{m}'' c_s(T_i - T_s^0)A_i}{V_c} + \frac{k_s A_i(T_i - T_s)}{L_s V_c}.$$

3.2 Gas Continuity Equation

Starting with the immersed boundary form of the gas continuity equation, (3), and splitting the time derivative terms yields

$$\alpha_g^0\frac{\rho-\rho^0}{\Delta t} + \rho\frac{\alpha_g - \alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_f \rho(\hat{u}\cdot\hat{A}_f)\alpha_f = \frac{\dot{m}'' A_i}{V_c}.$$

Setting the density time derivative to zero and substituting (1) for the volume fraction time derivative transforms the equation to

$$\frac{\dot{m}'' A_i}{V_c}\frac{\rho}{\rho_s} + \frac{1}{V_c}\sum_f \rho(\hat{u}\cdot\hat{A}_f)\alpha_f = \frac{\dot{m}'' A_i}{V_c}.$$

Rearranging this equation and defining the implicit and explicit source terms as $Sp_\rho = \dot{m}'' Ai/\rho_s V_c$ and $Su_\rho = \dot{m}'' Ai/V_c$ respectively further yields

$$\boxed{\frac{1}{V_c}\sum_f \rho(\hat{u}\cdot\hat{A}_f)\alpha_f = Su_\rho - Sp_\rho\rho.} \tag{10}$$

3.3 Gas Momentum Equation

Starting with the immersed boundary form of the gas momentum equation, (4), and splitting the time derivative yields

$$\hat{u}\frac{\rho\alpha_g - \rho^0\alpha_g^0}{\Delta t} + \rho^0\alpha_g^0\frac{\hat{u}-\hat{u}^0}{\Delta t} + \frac{1}{V_c}\sum_f \hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \frac{\hat{F}_p\alpha_f}{V_c} = S_{\hat{u}}\alpha_g. \tag{11}$$

Setting the velocity time derivative to zero and further splitting the density, volume fraction time derivative yields

$$\hat{u}\left(\alpha_g^0\frac{\rho-\rho^0}{\Delta t} + \rho\frac{\alpha_g-\alpha_g^0}{\Delta t}\right) + \frac{1}{V_c}\sum_f \hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \frac{\hat{F}_p\alpha_f}{V_c} = S_{\hat{u}}\alpha_g. \tag{12}$$

Again, assuming the density time derivative is zero and substituting (1) for the volume fraction derivative

$$\hat{u}\frac{\rho\dot{m}'' A_i}{\rho_s V_c} + \frac{1}{V_c}\sum_f \hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \frac{\hat{F}_p\alpha_f}{V_c} = S_{\hat{u}}\alpha_g. \tag{13}$$

Defining the implicit source term $Su_{\hat{u}} = \rho \dot{m}'' Ai/rho_s V_c$ and rearranging the equation leaves a final form of the momentum equation as

$$\boxed{\frac{1}{V_c}\sum_f \hat{u}(\rho\hat{u}\cdot\hat{A}_f)\alpha_f + \frac{\hat{F}_p\alpha_f}{V_c} = S_{\hat{u}}\alpha_g - Su_{\hat{u}}\hat{u}.} \tag{14}$$

3.4 Gas Energy Equation

Starting with the immersed boundary form of the gas energy equation and splitting the time derivative yields

$$\begin{aligned}
&\rho h_s\frac{\alpha_g - \alpha_g^0}{\Delta t} + \alpha_g^0\frac{\rho h_s - \rho^0 h_s^0}{\Delta t} + \frac{1}{V_c}\sum_f h_s(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{\rho K\alpha_g - \rho^0 K^0\alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_f K(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{p\alpha_g - p^0\alpha_g^0}{\Delta t} \\
=&S_E\alpha_g + Su_{t,g}.
\end{aligned}$$

Setting the density and sensible enthalpy time derivatives to zero and substituting (1) for the volume fraction time derivative leaves

$$\begin{aligned}
&h_s\frac{\rho\dot{m}''A_i}{\rho_s V_c} + \frac{1}{V_c}\sum_f h_s(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{\rho K\alpha_g - \rho^0 K^0\alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_f K(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{p\alpha_g - p^0\alpha_g^0}{\Delta t} \\
=&S_E\alpha_g + Su_{t,g}.
\end{aligned}$$

Defining the implicit source term as $Sp_{hs} = \rho\dot{m}'' Ai/rho_s V_c$ yields the final form of the equation

$$\boxed{\begin{aligned}
&\frac{1}{V_c}\sum_f h_s(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{\rho K\alpha_g - \rho^0 K^0\alpha_g^0}{\Delta t} + \frac{1}{V_c}\sum_f K(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{p\alpha_g - p^0\alpha_g^0}{\Delta t} \\
=&S_E\alpha_g + Su_{t,g} - Sp_{hs}h_s.
\end{aligned}} \tag{15}$$

3.5 Gas Species Equation

Starting with the immersed boundary form of the gas species equation and splitting the time derivative yields

$$\begin{aligned}
&\rho Y_i\frac{\alpha_g - \alpha_g^0}{\Delta t} + \alpha_g^0\frac{\rho Y_i - \rho^0 Y_i^0}{\Delta t} + \frac{1}{V_c}\sum_f Y_i(\rho\hat{u}\cdot\hat{A}_f)\alpha_f \\
+&\frac{1}{V_c}\sum_{f,g}(\hat{G}_i\cdot\hat{A}_f)\alpha_f = S_{Y_i}\alpha_g + \frac{Y_{i,b}\dot{m}''A_i}{V_c}
\end{aligned}$$

Setting the density and mass fraction time derivatives to zero and substituting (1) for the volume fraction time derivative leaves

$$Y_i \frac{\rho \dot{m}'' A_i}{\rho_s V_c} + \frac{1}{V_c} \sum_f Y_i (\rho \hat{u} \cdot \hat{A}_f) \alpha_f$$
$$+ \frac{1}{V_c} \sum_{f,g} (\hat{G}_i \cdot \hat{A}_f) \alpha_f = S_{Y_i} \alpha_g + \frac{Y_{i,b} \dot{m}'' A_i}{V_c}$$

Defining the implicit and explicit source terms as $Sp_{Yi} = \rho \dot{m}'' Ai / rho_s V_c$ and $Su_{Yi} = Y_{i,b} \dot{m}'' Ai / V_c$ respectively yields the final form of the equation

$$\boxed{\frac{1}{V_c} \sum_f Y_i (\rho \hat{u} \cdot \hat{A}_f) \alpha_f + \frac{1}{V_c} \sum_{f,g} (\hat{G}_i \cdot \hat{A}_f) \alpha_f = S_{Y_i} \alpha_g + Su_{Yi} - Sp_{Yi} Y_i} \tag{16}$$

Nomenclature

Symbols

A_i	interface area
A_s	solid phase frequency factor
c	specific heat capacity
D	species diffusivity
E	total energy
E_s	solid phase activation energy
$\hat{g}$	gravity vector
h_s	sensible enthalpy
K	kinetic energy
k	thermal conductivity
L	conduction length
M	molecular weight
$\dot{m}''$	mass flux
p	pressure
$\dot{Q}''$	heat flux
$\dot{Q}_g$	gas heat generation rate
Q_s	solid phase heat release
R	heat transfer resistance
$\bar{R}$	universal gas constant
$\dot{r}$	surface regression rate
S	volumetric source term
Sp	implicit source term
Su	explicit source term
T	temperature
t	time
$\hat{u}$	velocity vector
V	volume
Y	specie mass fraction
Y_b	specie mass fraction from solid combustion

Greek Symbols

α	volume fraction
$\dot{\Omega}$	species generation rate
ρ	density

Subscripts

c	cell
f	face
g	gas
i	interface
j	specie
s	solid
t	transferred

Superscripts

0	initial time value