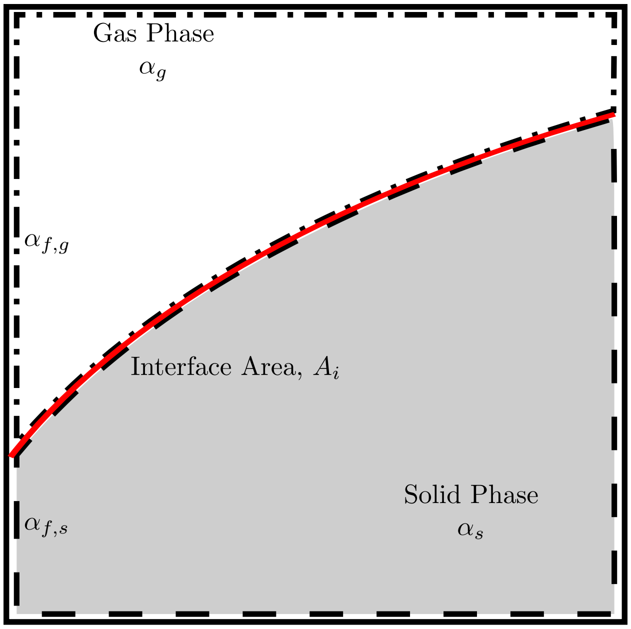

Figure 1: Diagram of Interface Cell

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 6.

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

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

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

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

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

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

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

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

Translate this to the full cell

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

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

$$\boxed{\frac{\rho \hat{u} \alpha_g - \rho^0 \hat{u}^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_{f} \hat{u}(\rho \hat{u} \cdot \hat{A}_f)\alpha_f + \frac{\hat{F}_p \alpha_f}{V_c} = S_{\hat{u}} \alpha_g + \frac{\hat{u}_b \dot{m}'' A_i}{V_c}} \tag{4}$$

4 Gas Energy Equation

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

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

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

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

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

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

Translate equation to full cell

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

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

$$
\boxed{
\begin{aligned}
&\frac{\rho h_s \alpha_g - \rho^0 h_s^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f h_s (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\
&+\frac{\rho K \alpha_g - \rho^0 K^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f K (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\
&+\frac{p \alpha_g - p^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f (\hat{q} \cdot \hat{A}_f) \alpha_f \\
&= S_E \alpha_g + \frac{K_b \dot{m}'' A_i}{V_c} + \frac{\hat{q}_b \cdot \hat{A}_b}{V_c}
\end{aligned}
} \tag{5}
$$

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

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

Translate this to the full cell

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

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

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

6 Cell Decomposition

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
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