1 Gas Continuity Equation

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

$$\frac{\partial}{\partial t} \int_{V_0} \rho dV + \int_{A_0} \rho(\hat{u} \cdot \hat{n}) dA = 0$$

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

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

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

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

2 Gas Momentum Equation

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

$$\frac{\partial}{\partial t} \int_{V_g} \rho \hat{\mathbf{u}} dV + \int_{A_g} \hat{u}(\rho \hat{u} \cdot \hat{n}) dA + \hat{F}_p = S(\hat{u})$$

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

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

Translate this to the full cell

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

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

$$\left[\frac{\rho \hat{u} \alpha_g - \rho^0 \hat{u}^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f \hat{u} (\rho \hat{u} \cdot \hat{A}_f) \alpha_f + \frac{\hat{F}_p \alpha_f}{V_c} = \frac{S(\hat{u})}{V_c} + \frac{\hat{u}_b \dot{m}'' A_b}{V_c} \right]$$
(2)

3 Gas Energy Equation

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

$$\frac{\partial}{\partial t} \int_{V_g} \rho E dV + \int_{A_g} (E + \frac{p}{\rho}) (\rho \hat{u} \cdot \hat{n}) dA + \int_{A_g} (\hat{q} \cdot \hat{n}) dA = S(E)$$

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

$$K = \frac{u^2 + v^2 + w^2}{2}$$

$$i = h_s - \frac{p}{\rho}$$

$$E = i + K$$

$$E = h_s + K - \frac{p}{\rho}$$

Substituting into the energy equation then yields

$$\frac{\partial}{\partial t} \int_{V_g} \rho(h_s + K - \frac{p}{\rho}) dV + \int_{A_g} (h_s + K)(\rho \hat{u} \cdot \hat{n}) dA + \int_{A_g} (\hat{q} \cdot \hat{n}) dA = S(E)$$

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

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

Translate equation to full cell

$$\begin{split} V_c \frac{\rho h_s \alpha_g - \rho^0 h_s^0 \alpha_g^0}{\Delta t} + \sum_f h_s (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\ + V_c \frac{\rho K \alpha_g - \rho^0 K^0 \alpha_g^0}{\Delta t} + \sum_f K (\rho \hat{u} \cdot \hat{A}_f) \alpha_f \\ + V_c \frac{\rho \alpha_g - \rho^0 \alpha_g^0}{\Delta t} + \sum_f (\hat{q} \cdot \hat{A}_f) \alpha_f \\ = S(E) + K_b \dot{m}'' A_b + \hat{q}_b \cdot \hat{A}_b \end{split}$$

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

$$\frac{\rho h_s \alpha_g - \rho^0 h_s^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f h_s (\rho \hat{u} \cdot \hat{A}_f) \alpha_f
+ \frac{\rho K \alpha_g - \rho^0 K^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f K (\rho \hat{u} \cdot \hat{A}_f) \alpha_f
+ \frac{p \alpha_g - p^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f (\hat{q} \cdot \hat{A}_f) \alpha_f
= \frac{S(E)}{V_c} + \frac{K_b \dot{m}'' A_b}{V_c} + \frac{\hat{q}_b \cdot \hat{A}_b}{V_c}$$
(3)

4 Gas Species Equation

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

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

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

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

Translate this to the full cell

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

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

$$\frac{\rho Y_i \alpha_g - \rho^0 Y_i^0 \alpha_g^0}{\Delta t} + \frac{1}{V_c} \sum_f Y_i (\rho \hat{u} \cdot \hat{A}_f) \alpha_f
+ \frac{1}{V_c} \sum_{f,g} (\hat{G}_i \cdot \hat{A}_f) \alpha_f = \frac{S(Y_i)}{V_c} + \frac{Y_{i,b} \dot{m}'' A_b}{V_c}$$
(4)