Scalar transport equations for multicomponent compressible flows and reacting flows

Cristopher Morales Ubal

c.m.ubal@gmail.com

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1 Derivation transport equation for Y_i

Let start considering the continuity equation given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \ , \tag{1}$$

On the other hand, we have the mass conservation for species i given by:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{u} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i \tag{2}$$

Using (1), the left-hand side of equation (2) can be rewritten as follows:

$$\begin{aligned}
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{u} Y_i) &= \rho \frac{\partial Y_i}{\partial t} + Y_i \frac{\partial \rho}{\partial t} + \rho \vec{u} \cdot \nabla Y_i + Y_i \nabla \cdot \rho \vec{u} && (3)\\
&= \rho \left(\frac{\partial Y_i}{\partial t} + \vec{u} \cdot \nabla Y_i \right) + Y_i \underbrace{\left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) \right)}_{=0} && (4)\\
&= \rho \left(\frac{\partial Y_i}{\partial t} + \vec{u} \cdot \nabla Y_i \right) && (5)
\end{aligned}$$

Then replacing (5) in (2), we have:

$$\begin{aligned}
\rho \left(\frac{\partial Y_i}{\partial t} + \vec{u} \cdot \nabla Y_i \right) &= \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i && (6)\\
\iff \frac{\partial Y_i}{\partial t} + \vec{u} \cdot \nabla Y_i &= \frac{1}{\rho} \nabla \cdot (\rho D_i \nabla Y_i) + \frac{\dot{\omega}_i}{\rho} && (7)
\end{aligned}$$

On the other hand, using derivation rules, the convective term on the left-hand side of (7) can be expressed as:

$$\vec{u} \cdot \nabla Y_i = \nabla \cdot (\vec{u} Y_i) - Y_i \nabla \cdot \vec{u} \tag{8}$$

Then, equation (7) can be written as follows:

$$\frac{\partial Y_i}{\partial t} + \cdot \nabla \cdot (Y_i \vec{u}) = \frac{1}{\rho} \nabla \cdot (\rho D_i \nabla Y_i) + \frac{\dot{\omega}_i}{\rho} + Y_i \nabla \cdot \vec{u} \tag{9}$$

Finally, the diffusion term can be rewritten as:

$$\frac{1}{\rho} \nabla \cdot (\rho D_i \nabla Y_i) = \nabla \cdot (D_i \nabla Y_i) + \frac{D_i}{\rho} \nabla \rho \cdot \nabla Y_i \tag{10}$$

Therefore, a transport equation for Y_i is given by:

$$\frac{\partial Y_i}{\partial t} + \cdot \nabla \cdot (Y_i \vec{u}) = \nabla \cdot (D_i \nabla Y_i) + \frac{\dot{\omega}_i}{\rho} + Y_i \nabla \cdot \vec{u} + \frac{D_i}{\rho} \nabla \rho \cdot \nabla Y_i \tag{11}$$

2 Derivation transport equation for $\mathcal{Y}_i = \rho Y_i$.

The mass conservation for species i (2) can be expressed in terms of the transport scalar variable $\mathcal{Y}_i = \rho Y_i$ as follows:

$$\frac{\partial \mathcal{Y}_i}{\partial t} + \nabla \cdot (\vec{u} \mathcal{Y}_i) = \nabla \cdot \left(\rho D_i \nabla \left(\frac{\mathcal{Y}_i}{\rho} \right) \right) + \dot{\omega}_i \tag{12}$$

On the right-hand side, the diffusion term can be expressed as follows:

$$\rho D_i \nabla \left(\frac{\mathcal{Y}_i}{\rho} \right) = D_i \nabla \mathcal{Y}_i - \frac{D_i \mathcal{Y}_i}{\rho} \nabla \rho \tag{13}$$

Therefore, replacing (13) in (12), we obtain:

$$\frac{\partial \mathcal{Y}_i}{\partial t} + \nabla \cdot (\vec{u} \mathcal{Y}_i) = \nabla \cdot \left(D_i \nabla \mathcal{Y}_i - \frac{D_i \mathcal{Y}_i}{\rho} \nabla \rho \right) + \dot{\omega}_i \tag{14}$$

Finally, it must be noted that, using (14), we solve for $\mathcal{Y}_i$ and then reconstruct the species mass fraction Y_i at each node as follows:

$$Y_i = \frac{\mathcal{Y}_i}{\rho} \tag{15}$$