

Flux Transformation Matrices

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Consider the $n - 1$ dimensional transformations:

$$(\mathbf{j}) = [B^{ou}](\mathbf{j}^u), \quad (1)$$

$$(\mathbf{j}^u) = [B^{uo}](\mathbf{j}), \quad (2)$$

where $[B^{uo}] = [B^{ou}]^{-1}$. In class, we derived an expression for $[B^{ou}]$. Here we will derive the expression for $[B^{uo}]$.

Let's look at the expression for the mass diffusion flux relative to a molar-averaged velocity:

$$\begin{aligned} \mathbf{j}_i^u &= \rho_i(\mathbf{u}_i - \mathbf{u}), \\ &= \rho_i(\mathbf{u}_i - \mathbf{v}) + \rho_i(\mathbf{v} - \mathbf{u}), \\ &= \mathbf{j}_i + \rho_i(\mathbf{v} - \mathbf{u}). \end{aligned} \quad (3)$$

Since our goal is to express \mathbf{j}_i in terms of \mathbf{j}_i^u , we have rearranged the expression for \mathbf{j}_i^u in terms of \mathbf{j}_i and another term: $\rho_i(\mathbf{v} - \mathbf{u})$. Now let's see if we can use the expression for \mathbf{j}_i to eliminate the $(\mathbf{u} - \mathbf{v})$ term from (3). Recall

$$\mathbf{j}_i = \rho_i(\mathbf{u}_i - \mathbf{v}). \quad (4)$$

This isn't useful to us since it has a \mathbf{u}_i in it. Note, however, that if we sum this, we obtain $\sum_{i=1}^n \mathbf{j}_i = 0$. This is also not useful. Recall we need a term like $\rho_i(\mathbf{u} - \mathbf{v})$. Recall that $\mathbf{u} = \sum_{i=1}^n x_i \mathbf{u}_i$. Look closely at (4). If we multiply by x_i/ω_i then we have

$$\frac{x_i}{\omega_i} \mathbf{j}_i = \rho x_i(\mathbf{u}_i - \mathbf{v}).$$

Now if we sum this, we should get a \mathbf{u} from the $x_i \mathbf{u}_i$ term:

$$\begin{aligned} \sum_{i=1}^n \frac{x_i}{\omega_i} \mathbf{j}_i &= \rho \sum_{i=1}^n x_i \mathbf{u}_i - \rho \mathbf{v}, \\ &= \rho(\mathbf{u} - \mathbf{v}), \\ \frac{1}{\rho} \sum_{i=1}^n \frac{x_i}{\omega_i} \mathbf{j}_i &= \mathbf{u} - \mathbf{v}. \end{aligned} \quad (5)$$

Great! Now we are ready to return to equation (3). Substituting (5) into (3) gives

$$\begin{aligned}
 \mathbf{j}_i^u &= \mathbf{j}_i - \frac{\rho_i}{\rho} \sum_{j=1}^n \frac{x_j}{\omega_j} \mathbf{j}_j, \\
 &= \mathbf{j}_i - \omega_i \left(\sum_{j=1}^{n-1} \frac{x_j}{\omega_j} \mathbf{j}_j + \frac{x_n}{\omega_n} \mathbf{j}_n \right), \\
 &= \mathbf{j}_i - \omega_i \left(\sum_{j=1}^{n-1} \frac{x_j}{\omega_j} \mathbf{j}_j - \frac{x_n}{\omega_n} \sum_{j=1}^{n-1} \mathbf{j}_j \right), \\
 &= \mathbf{j}_i - \sum_{j=1}^{n-1} \omega_i \left(\frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right) \mathbf{j}_j, \\
 &= \sum_{j=1}^{n-1} \left(\delta_{ij} - \omega_i \left(\frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right) \right) \mathbf{j}_j, \\
 (\mathbf{j}^u) &= [B^{u0}](\mathbf{j}),
 \end{aligned}$$

with

$$B_{ij}^{u0} = \delta_{ij} - \omega_i \left(\frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right).$$

This is equation 1.2.25 in Taylor & Krishna.