Flux Transformation Matrices

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Consider the \( n - 1 \) dimensional transformations:

\[
\begin{align*}
  (j) &= [B^{ou}](j^u), \\
  (j^u) &= [B^{uo}](j),
\end{align*}
\]

(1)

(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:

\[
\begin{align*}
  j_i^u &= \rho_i(u_i - u), \\
         &= \rho_i(u_i - v) + \rho_i(v - u), \\
         &= j_i + \rho_i(v - u).
\end{align*}
\]

(3)

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

\[
  j_i = \rho_i(u_i - v).
\]

(4)

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

\[
\frac{x_i}{\omega_i} j_i = \rho x_i(u_i - v).
\]

Now if we sum this, we should get a \( u \) from the \( x_i u_i \) term:

\[
\begin{align*}
  \sum_{i=1}^{n} \frac{x_i}{\omega_i} j_i &= \rho \sum_{i=1}^{n} x_i u_i - \rho v, \\
                               &= \rho(u - v), \\
  \frac{1}{\rho} \sum_{i=1}^{n} \frac{x_i}{\omega_i} j_i &= u - v.
\end{align*}
\]

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

\[ j^u = j_i - \frac{\rho_i}{\rho} \sum_{j=1}^{n} \frac{x_j}{\omega_j} j_j \]

\[ = j_i - \omega_i \left( \sum_{j=1}^{n-1} \frac{x_j}{\omega_j} j_j + \frac{x_n}{\omega_n} j_n \right), \]

\[ = j_i - \omega_i \left( \sum_{j=1}^{n-1} \frac{x_j}{\omega_j} j_j - \frac{x_n}{\omega_n} \sum_{j=1}^{n-1} j_j \right), \]

\[ = j_i - \sum_{j=1}^{n-1} \omega_i \left( \frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right) j_j, \]

\[ = \sum_{j=1}^{n-1} \left( \delta_{ij} - \omega_i \left( \frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right) \right) j_j, \]

\[ (j^u) = [B^{ij}] (j), \]

with

\[ B^{ij} = \delta_{ij} - \omega_i \left( \frac{x_j}{\omega_j} - \frac{x_n}{\omega_n} \right). \]

This is equation 1.2.25 in Taylor & Krishna.