GMS Equations From
Irreversible
Thermodynamics

ChEn 6603

References

Outline

Entropy, Entropy transport

Entropy production: “forces” & “fluxes”
  • Species diffusive fluxes & the Generalized Maxwell-Stefan Equations
  • Heat flux
  • Thermodynamic nonidealities & the “Thermodynamic Factor”

Example: the ultracentrifuge

Fick’s law (the full version)

Review
A Perspective

Reference velocities
• Allows us to separate a species flux into convective and diffusive components.

Governing equations
• Describe conservation of mass, momentum, energy at the continuum scale.

GMS equations
• Provide a general relationship between species diffusion fluxes and diffusion driving force(s).
• So far, we’ve assumed:
  ‣ Ideal mixtures (inelastic collisions)
  ‣ “small” pressure gradients

Goal: obtain a more general form of the GMS equations that represents more physics
• Body forces acting differently on different species (e.g. electromagnetic fields)
• Nonideal mixtures
• Large pressure gradients (centrifugal separations)
Entropy

Entropy differential: \[ Tds = de + pdv - \sum_{i=1}^{n} \tilde{\mu}_i d\omega_i \]

Total (substantial/material) derivative: \[ \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + v \cdot \nabla \]

\[ T\rho \frac{Ds}{Dt} = \rho \frac{De}{Dt} + p\rho \frac{Dv}{Dt} - \sum_{i=1}^{n} \tilde{\mu}_i \rho \frac{D\omega_i}{Dt} \]

\[ \rho = 1/v \]

\[ T\rho \frac{Ds}{Dt} = \rho \frac{De}{Dt} - \frac{p}{\rho} \frac{D\rho}{Dt} - \sum_{i=1}^{n} \tilde{\mu}_i \rho \frac{D\omega_i}{Dt} \]

\[ \rho \frac{De}{Dt} = -\nabla \cdot \mathbf{q} - \tau : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} + \sum_{i=1}^{n} \mathbf{f}_i \cdot \mathbf{j}_i \]

\[ \frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} \]

\[ \rho \frac{D\omega_i}{Dt} = -\nabla \cdot \mathbf{j}_i + \sigma_i \]
Entropy Transport

\[
T \rho \frac{D s}{D t} = -\nabla \cdot q - \tau : \nabla v - \rho \nabla \cdot v + \sum_{i=1}^{n} f_i \cdot j_i + \frac{p}{\rho} \nabla \cdot v - \sum_{i=1}^{n} \tilde{\mu}_i (-\nabla \cdot j_i + \sigma_i),
\]

\[
\rho \frac{D s}{D t} = -\nabla \cdot \left[ \frac{1}{T} \left( q - \sum_{i=1}^{n} \tilde{\mu}_i j_i \right) \right] + q \cdot \nabla \left( \frac{1}{T} \right) - \sum_{i=1}^{n} j_i \cdot \nabla \left( \frac{\tilde{\mu}_i}{T} \right) - \frac{1}{T} \tau : \nabla v + \frac{1}{T} \sum_{i=1}^{n} f_i \cdot j_i - \frac{1}{T} \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i.
\]

\(\nabla (\alpha \beta) = \alpha \nabla \beta + \beta \nabla \alpha\)

Transport of \(s\)  
Production of \(s\)
\[
\frac{\rho D_s}{Dt} = -\nabla \left[ \frac{1}{T} \left( q - \sum_{i=1}^{n} \tilde{\mu}_i j_i \right) \right] + q \cdot \nabla \left( \frac{1}{T} \right) - \sum_{i=1}^{n} j_i \cdot \nabla \left( \frac{\tilde{\mu}_i}{T} \right) - \frac{1}{T} \tau : \nabla \mathbf{v} + \frac{1}{T} \sum_{i=1}^{n} f_i \cdot j_i - \frac{1}{T} \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i
\]

Transport of \( s \)

Production of \( s \)

Now let’s write this in the form:

\[
\frac{D_s}{Dt} = -\nabla \cdot j_s + \sigma_s
\]

diffusive transport of entropy

\[
\begin{align*}
\sigma_s &= q \cdot \nabla \left( \frac{1}{T} \right) - \sum_{i=1}^{n} j_i \cdot \nabla \left( \frac{\tilde{\mu}_i}{T} \right) - \frac{1}{T} \tau : \nabla \mathbf{v} + \frac{1}{T} \sum_{i=1}^{n} f_i \cdot j_i - \frac{1}{T} \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i, \\
&= -\frac{q}{T} \cdot \nabla \ln T - \sum_{i=1}^{n} j_i \cdot \left[ \nabla \left( \frac{\tilde{\mu}_i}{T} \right) - \frac{1}{T} f_i \right] - \frac{1}{T} \tau : \nabla \mathbf{v} - \frac{1}{T} \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i
\end{align*}
\]

Note that we haven’t “completed” the chain rule here. We will apply it to species later...

\[
\nabla \left( \frac{\tilde{\mu}_i}{T} \right) = \frac{\partial \tilde{\mu}_i}{\partial T} \nabla \left( \frac{T}{T} \right) + \frac{1}{T} \frac{\partial \tilde{\mu}_i}{\partial p} \nabla p + \frac{1}{T} \nabla_{T,p} \tilde{\mu}_i,
\]

\[
= \frac{1}{T} \left( \frac{1}{M_i} \frac{\partial \mu_i}{\partial p} \nabla p + \nabla_{T,p} \tilde{\mu}_i \right),
\]

\[
= \frac{1}{T} \left( \frac{\bar{V}_i}{M_i} \nabla p + \nabla_{T,p} \tilde{\mu}_i \right)
\]

\[
T \sigma_s = -q \cdot \nabla \ln T - \sum_{i=1}^{n} j_i \cdot \left[ \nabla_{T,p} \tilde{\mu}_i + \frac{\bar{V}_i}{M_i} \nabla p - f_i \right] - \tau : \nabla \mathbf{v} - \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i
\]

(entropy production due to species diffusion)
Part of the Entropy Source Term...

\[ \sum_{i=1}^{n} \mathbf{j}_i \cdot \left[ \nabla_{T,p} \tilde{\mu}_i + \frac{\bar{V}_i}{M_i} \nabla p - \mathbf{f}_i \right] = \sum_{i=1}^{n} \mathbf{j}_i \cdot \left( \Lambda_i - \frac{1}{\rho} \nabla p + \sum_{k=1}^{n} \omega_k \mathbf{f}_k \right) \]

Why can we add this “arbitrary” term? What does this term represent?

\[ \sum_{i=1}^{n} \mathbf{j}_i \cdot \Lambda_i = \sum_{i=1}^{n} \left( \rho \omega_i (\mathbf{u}_i - \mathbf{v}) \cdot \left[ \nabla_{T,p} \tilde{\mu}_i + \left( \frac{\bar{V}_i}{M_i} - \frac{1}{\rho} \right) \nabla p - \mathbf{f}_i + \sum_{k=1}^{n} \omega_k \mathbf{f}_k \right] \right) = \sum_{i=1}^{n} \left( \mathbf{u}_i - \mathbf{v} \right) \cdot \left[ c_i \nabla_{T,p} \mu_i + (\phi_i - \omega_i) \nabla p - \rho \omega_i \left( \mathbf{f}_i - \sum_{k=1}^{n} \omega_k \mathbf{f}_k \right) \right] = cRT \sum_{i=1}^{n} \mathbf{d}_i \cdot (\mathbf{u}_i - \mathbf{v}) = cRT \sum_{i=1}^{n} \frac{1}{\rho \omega_i} \mathbf{d}_i \cdot \mathbf{j}_i \]

\[ cRT \mathbf{d}_i = c_i \nabla_{T,p} \mu_i + (\phi_i - \omega_i) \nabla p - \omega_i \rho \left( \mathbf{f}_i - \sum_{k=1}^{n} \omega_k \mathbf{f}_k \right) \]

From physical reasoning (recall \( \mathbf{d}_i \) represents force per unit volume driving diffusion) or the Gibbs-Duhem equation,

\[ \sum_{i=1}^{n} \mathbf{d}_i = 0 \]
The Entropy Source Term - Summary

\[ \rho \frac{Ds}{Dt} = -\nabla \cdot \mathbf{j}_s + \sigma_s \]

\[ \mathbf{j}_s = \frac{1}{T} \left( \mathbf{q} - \sum_{i=1}^{n} \tilde{\mu}_i \mathbf{j}_i \right) \]

From the previous slide:

\[ \sum_{i=1}^{n} \mathbf{j}_i \cdot \Lambda_i = cRT \sum_{i=1}^{n} \frac{\mathbf{d}_i \cdot \mathbf{j}_i}{\rho_i} \]

\[ cRT \mathbf{d}_i = c_i \nabla T, p \mu_i + (\phi_i - \omega_i) \nabla p - \omega_i \rho \left( \mathbf{f}_i - \sum_{k=1}^{n} \omega_k \mathbf{f}_k \right) \]

\[ T \sigma_s = -\mathbf{q} \cdot \nabla \ln T - \sum_{i=1}^{n} \mathbf{j}_i \cdot \left[ \nabla T, p \tilde{\mu}_i + \frac{\tilde{V}_i}{M_i} \nabla p - \mathbf{f}_i \right] \rightarrow \mathbf{\Lambda}_i \]

\[ = -\mathbf{q} \cdot \nabla \ln T - \sum_{i=1}^{n} \frac{cRT}{\rho_i} \mathbf{d}_i \cdot \mathbf{j}_i - \mathbf{\tau} : \nabla \mathbf{v} - \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i \]

Interpretation of each term???
\[ \sigma_s \sim \text{Forces} \cdot \text{Fluxes} \]

\[ T\sigma_s = -q \cdot \nabla \ln T - \sum_{i=1}^{n} \frac{cRT}{\rho_i} \mathbf{d}_i \cdot \mathbf{j}_i - \tau : \nabla \mathbf{v} - \sum_{i=1}^{n} \tilde{\mu}_i \sigma_i \]

**Fundamental principle of irreversible thermodynamics:**

\[ \sigma_s = \sum_{\alpha} J_{\alpha} F_{\alpha} \]

<table>
<thead>
<tr>
<th>Flux, ( J_{\alpha} )</th>
<th>Force, ( F_{\alpha} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q )</td>
<td>(-\nabla \ln T)</td>
</tr>
<tr>
<td>( \mathbf{j}_i )</td>
<td>(-\frac{cRT}{\rho_i} \mathbf{d}_i)</td>
</tr>
<tr>
<td>( \tau )</td>
<td>(-\nabla \mathbf{v})</td>
</tr>
</tbody>
</table>

**Fluxes are functions of:**

- Thermodynamic state variables: \( T, p, \omega_i \).
- **Forces of same tensorial order** (Curie's postulate)
  - What does this mean?
  - More soon…

\[ J_{\alpha} = J_{\alpha}(F_1, F_2, \ldots, F_\beta; T, p, \omega_i) \]

\[ J_{\alpha} = \sum_{\beta} \left( \frac{\partial J_{\alpha}}{\partial F_\beta} \right) F_\beta + \mathcal{O}(F_\beta F_\gamma) \]

\[ \approx \sum_{\beta} L_{\alpha\beta} F_\beta \]

\[ L_{\alpha\beta} = \frac{\partial J_{\alpha}}{\partial F_\beta} \]

\[ L_{\alpha\beta} = L_{\beta\alpha} \]

\( L_{\alpha\beta} \) - Onsager (phenomenological) coefficients
Species Diffusive Fluxes

Tensorial order of “1” ⇒ any vector force may contribute.

<table>
<thead>
<tr>
<th>Flux: $J_\alpha$</th>
<th>$\mathbf{q}$</th>
<th>$\mathbf{j}_i$</th>
<th>$\mathbf{\tau}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Force: $F_\alpha$</td>
<td>$-\nabla \ln T$</td>
<td>$-\frac{cRT}{\rho_i} \mathbf{d}_i$</td>
<td>$-\nabla \mathbf{v}$</td>
</tr>
</tbody>
</table>

**Index form:**

From irreversible thermo:

$$\mathbf{j}_i = - \sum_{j=1}^{n-1} L_{ij} \frac{cRT}{\rho_j} \mathbf{d}_j - L_i q \nabla \ln T$$

**Fick’s Law:**

$$\mathbf{j}_i = -\rho \sum_{j=1}^{n-1} D_{ij} \mathbf{d}_j - D_i^T \nabla \ln T$$

$D_{ij}$ - Fickian diffusivity

$D_i^T$ - Thermal Diffusivity

**Generalized Maxwell-Stefan Equations:**

$$\mathbf{d}_i = -\sum_{j\neq i}^n \frac{x_i x_j}{\rho D_{ij}} \left( \frac{\mathbf{j}_i}{\omega_i} - \frac{\mathbf{j}_j}{\omega_j} \right) - \nabla \ln T \sum_{j \neq i}^n x_i x_j \alpha_{ij}^T$$

$$\rho(\mathbf{d}) = -[B^{on}](\mathbf{j}) - \nabla \ln T \mathbf{\Gamma}(D^T)$$

where

$$\alpha_{ij}^T = \frac{1}{D_{ij}} \left( \frac{D_i^T}{\rho_i} - \frac{D_j^T}{\rho_j} \right)$$
Constitutive Law: Heat Flux

Tensorial order of “1” ⇒ any vector force may contribute.

\[ q = -L_{qq} \nabla \ln T - \sum_{i=1}^{n} L_{qi} \frac{cRT}{\rho_i} d_i \]

Choose \( L_{qq} = \lambda T \) to obtain “Fourier’s Law”

“Dufour” effect - mass driving force can cause heat flux! Usually neglected.

\[ q = -\lambda \nabla T + \sum_{i=1}^{n} h_i j_i + \sum_{i=1}^{n} \sum_{j \neq i} \frac{cRT D_{ij} x_i x_j}{\rho_i \rho_j} \left( \frac{j_i}{\rho_i} - \frac{j_j}{\rho_j} \right) \]

The “Species” term is typically included here, even though it does not come from irreversible thermodynamics. Occasionally radiative terms are also included here...

Note: the Dufour effect is usually neglected.
Observations on the GMS Equations

\[ d_i = \sum_{j=1}^{n} \frac{x_i J_j - x_j J_i}{cD_{ij}} - \nabla \ln T \sum_{j=1}^{n} x_i x_j \alpha_{ij}^T \]

\[ cRTd_i = c_i \nabla_{T,p} \mu_i + (\phi_i - \omega_i) \nabla p - \omega_i \rho \left( f_i - \sum_{k=1}^{n} \omega_k f_k \right) \]

What have we gained?
- Thermal diffusion (Soret/Dufuor) & its origins.
  - Typically neglected.
- “Full” diffusion driving force
  - Chemical potential gradient (rather than mole fraction). More later.
  - Pressure driving force.
    - When will \( \phi_i \neq \omega_i \)? More later.
  - Body force term.
    - Does gravity enter here?

Onsager coefficients themselves not too important from a “practical” point of view.
Still don’t know how to get the binary diffusivities.
The Thermodynamic Factor, $\Gamma$

$$d_i = \frac{x_i}{RT} \nabla_{T,p} \mu_i + \frac{1}{c_t RT} (\phi_i - \omega_i) \nabla p - \frac{\rho_i}{c_t RT} \left( f_i - \sum_{k=1}^{n} \omega_k f_k \right)$$

$$\mu_i = \mu_i(T, p, x_j)$$

$$\nabla_{T,p} \mu_i = \sum_{j=1}^{n-1} \frac{\partial \mu_i}{\partial x_j} \bigg|_{T,p,\Sigma} \nabla x_j$$

$$\mu_i(T, p) = \mu_i^0 + RT \ln \gamma_i x_i$$

$$\gamma - \text{Activity coefficient}$$

Many models available (see T&K Appendix D)

$$\Gamma_{ij} \equiv \delta_{ij} + x_i \frac{\partial \ln \gamma_i}{\partial x_j} \bigg|_{T,p,\Sigma}$$

$$d_i = \sum_{j=1}^{n-1} \Gamma_{ij} \nabla x_j + \frac{1}{c_t RT} (\phi_i - \omega_i) \nabla p - \frac{\rho_i}{c_t RT} \left( f_i - \sum_{k=1}^{n} \omega_k f_k \right)$$

Note: for ideal gas, $p = c_t RT$
Example: The Ultracentrifuge

Used for separating mixtures based on components’ molecular weight.

Consider a closed system...

-depleted in dense species

\[
f = f_i = \Omega^2 r
\]

For a closed centrifuge (no flow) with a known initial charge, what is the equilibrium species profile?
Species equations: \[
\frac{\partial \rho_i}{\partial t} = -\nabla \cdot \mathbf{n}_i + s_i \quad \text{steady, 1D, no reaction} \quad \frac{\partial n_i}{\partial r} = 0
\]
\[
n_i = \rho_i v_r + j_{i,r} = 0 \quad \Rightarrow \quad j_{i,r} = J_{i,r} = 0
\]

GMS Equations: \[
d_i = \sum_{j=1}^{n} \frac{x_i J_j - x_j J_i}{cD_{ij}} = 0
\]
The generalized diffusion driving force:
\[
d_i = \sum_{j=1}^{n-1} \Gamma_{ij} \nabla x_j + \frac{1}{c_t RT} (\phi_i - \omega_i) \nabla p - \frac{\omega_i \rho}{c_t RT} \left( f_i - \sum_{k=1}^{n} \omega_k f_k \right)
\]
\[
0 = \sum_{j=1}^{n-1} \Gamma_{ij} \frac{dx_j}{dr} + \frac{1}{c_t RT} (\phi_i - \omega_i) \frac{dp}{dr} - \frac{\omega_i \rho}{c_t RT} \left( \Omega^2 r - \sum_{k=1}^{n} \omega_k \Omega^2 r \right)
\]
\[
\sum_{j=1}^{n-1} \Gamma_{ij} \frac{dx_j}{dr} = \frac{1}{c_t RT} (\omega_i - \phi_i) \frac{dp}{dr}
\]

For an ideal gas mixture, \( \phi_i = x_i \), and \( \Gamma_{ij} = \delta_{ij} \).
\[
\frac{dx_i}{dr} = \frac{1}{c_t RT} (\omega_i - x_i) \frac{dp}{dr}
\]

We don’t know \( dp/dr \) or \( x_{i0} \) (composition at \( r = 0 \)).
Species mole balance:

\[ \int_{0}^{r_L} c x_i 2\pi r \, dr = \int_{0}^{r_L} c^* x^*_i 2\pi r \, dr \]

For species \( i \),

\[ \int_{0}^{r_L} p x_i r \, dr = p^* x^*_i \frac{r^2_L}{2} \]

* indicates the initial condition (pure stream).

Must know \( p(r) \) and \( x_i(r) \) to integrate this.

Species mole balance constrains the species profile solution (dictates the species boundary condition)

Momentum:

\[ \frac{\partial \rho \mathbf{v}}{\partial t} = - \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \nabla \cdot \mathbf{\tau} - \nabla p + \rho \sum_{i=1}^{n} \omega_i \mathbf{f}_i \]

at steady state (no flow):

\[ \frac{dp}{dr} = \rho \sum_{i=1}^{n} \omega_i f_{r,i} = \rho \Omega^2 r \]

\[ \frac{dp}{dr} = \rho \Omega^2 r = \frac{pM}{RT} \Omega^2 r \]

We don’t know \( p_0 \) (pressure at \( r = 0 \)).

The momentum equation gives the pressure profile, but is coupled to the species equations through \( M \).
Total mole balance (at equilibrium):

\[
\int_V c \, dV = \int_V c^* \, dV \quad * \text{ indicates the initial condition (pure stream).}
\]

\[
\int_0^{r_L} cr \, dr = c^* \frac{r_L^2}{2}
\]

\[
dV = L2\pi rdr \quad c = \frac{p}{RT}
\]

\[
\int_0^{r_L} pr \, dr = p^* \frac{r_L^2}{2}
\]

Substitute \( p(r) \) and solve this for \( p_0 \)...

Total mole balance constrains the pressure solution (dictates the pressure boundary condition)

---

Solve these equations:

\[
\frac{dx_i}{dr} = \frac{M}{RT} (\omega_i - x_i) \Omega^2 r
\]

\[
\frac{dp}{dr} = \rho \Omega^2 r = \frac{pM}{RT} \Omega^2 r
\]

With these constraints:

\[
\int_0^{r_L} p x_i r \, dr = p^* x_i^* \frac{r_L^2}{2}
\]

\[
\int_0^{r_L} pr \, dr = p^* \frac{r_L^2}{2}
\]

Note: \( M \) couples all of the equations together and makes them nonlinear.

---

Option A:

1. Guess \( x_{i0}, p_0 \).
2. Numerically solve the ODEs for \( x_i, p \).
3. Are the constraints met? If not, return to step 1.

Option B:

Try to simplify the problem by making approximations.

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Note: for tips on solving ODEs numerically in Matlab, see my wiki page.
Example: separation of Air into $N_2, O_2$.

- Centrifuge diameter: 20 cm
- Air initially at STP

Approximation Level 1

- Approximate $M$ as constant, $(M_{O_2} + M_{N_2})/2$, for the pressure equation only. This decouples the pressure solution from the species and gives an easy analytic solution for pressure profile.
- Solve species equations numerically, given the analytic pressure profile.

Approximation Level 2

- Approximate $M$ as constant, $(M_{O_2} + M_{N_2})/2$, for the species and pressure equations.
- Obtain a fully analytic solution for both species and pressure.

**Graphs:**
- Left graph shows $p$ (atm) vs. $r$ (m) for different RPMs.
- Right graph shows $O_2$ Mole Fraction vs. $r$ (m) for different RPMs.

Legend:
- Blue: fully numeric
- Green: constant $M$
- Red: approximate 1
- Dashed Red: approximate 2
Fick’s Law (revisited)

Ignoring thermal diffusion,

\[ \vec{d}_i = - \sum_{j=1}^{n} \frac{x_i x_j}{\rho D_{ij}} \left( \frac{j_i}{\omega_i} - \frac{j_j}{\omega_j} \right) - \nabla \ln T \sum_{j=1}^{n} x_i x_j \alpha_{i,j}^T \]

\[ = - \sum_{j=1}^{n} \frac{x_j \vec{J}_i - x_i \vec{J}_j}{c D_{ij}} - \nabla \ln T \sum_{j=1}^{n} x_i x_j \alpha_{i,j}^T \]

\[ \vec{d}_i = \sum_{j=1}^{n-1} \Gamma_{ij} \nabla x_j + \frac{1}{c_t RT} (\phi_i - \omega_i) \nabla p - \frac{\rho_i}{c_t RT} \left( \vec{f}_i - \sum_{k=1}^{n} \omega_k \vec{f}_k \right) \]

\[ \vec{J} = -c[B]^{-1}(\vec{d}) - \nabla \ln T(D^T) \]

This is the same \([B]\) matrix as before (T&K eq. 2.1.21-2.1.22)

Ignoring thermal diffusion,

\[ (\vec{J}) = -c[B]^{-1}[\Gamma](\nabla x) - \frac{\nabla p}{RT} [B]^{-1} ((\phi) - (\omega)) - \frac{\rho}{RT} [B]^{-1} [\omega] ((\vec{f}) - [\omega](\vec{f} + \vec{f}_n)) \]

Notes: \([D]=[B]^{-1}[\Gamma]\)

For ideal mixtures: \([\Gamma]=[I]\)

In the binary case: \(D_{11}=\Gamma_{11} D_{12}\)

How do we interpret each term?
When is each term important?

\[ \text{Notes: } [D]=\Gamma^{-1}[\Gamma] \]

For ideal mixtures: \([\Gamma]=[I]\)

In the binary case: \(D_{11}=\Gamma_{11} D_{12}\)
Accomplishments

- Defined “reference velocities” and “diffusion fluxes”
- Governing equations for multicomponent, reacting flow.
  - mass-averaged velocity…
- Established a rigorous way to compute the diffusive fluxes from first principles.
  - Can handle diffusion in systems of arbitrary complexity, including:
    - nonideal mixtures, EM fields, large pressure & temperature gradients, multiple species, chemical reaction, etc.
- Simplifications for ideal mixtures, negligible pressure gradients, etc.
- Solutions for “simple” problems.

Still Missing:

- Models for binary diffusivities.
  - Given a model, we are good to go!

Roadmap:

- Models for binary diffusivities. (T&K Chapter 4) - we won’t cover this...
- Simplified models for multicomponent diffusion
- Interphase mass transfer (surface discontinuities)
- Turbulence - models for diffusion in turbulent flow.
- Combined heat, mass, momentum transfer.