Outline

Simplified Models for Interphase Mass Transfer

- Interphase mass transfer
  - Mass balances at interfaces (phase boundaries, etc)
  - Mass transfer coefficients
- Film Theory
  - gives us insight into defining mass transfer coefficients for a very specific case...
- The "Bootstrap Problem"
  - given diffusive fluxes, can we find the total fluxes?
- Solution procedure - Film Theory

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Interphase Mass Transfer

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Interface Balance Equations

Generic transport equation (mass-averaged velocity):

$$\frac{\partial \rho_t \Psi}{\partial t} + \nabla \cdot (\rho_t \Psi \mathbf{v}) + \nabla \cdot \mathbf{\Phi} = \zeta$$

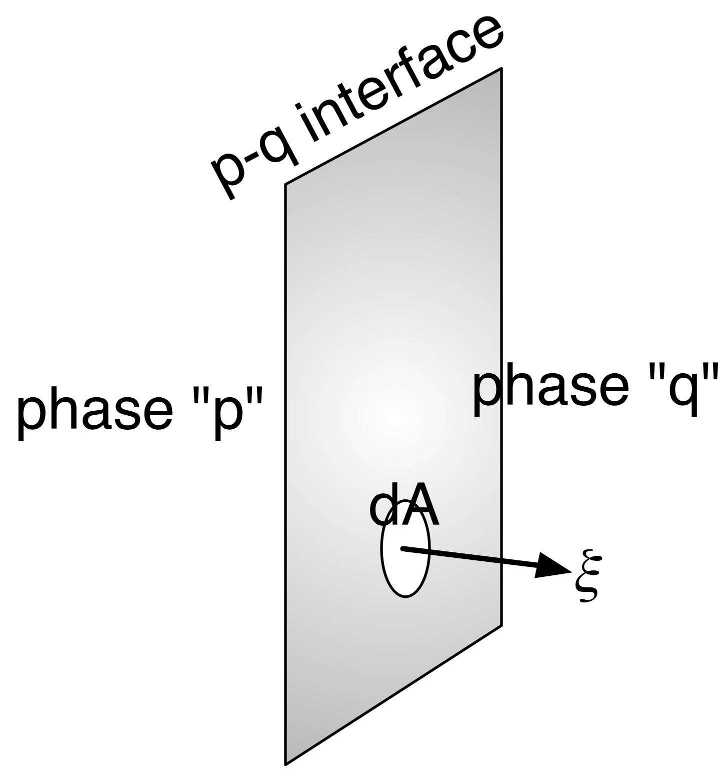
Assumes that Ψ is a continuous function.

Concept: solve the governing equations in each phase, and connect them with an appropriate balance at the interface (boundary condition).

Balance at the interface surface

$$\int_S \underbrace{\left(\mathbf{\Phi}^q + \rho_t^q \Psi^q (\mathbf{v}^q - \mathbf{u}^I)\right) \cdot \xi}_{\text{Flux of } \Psi \text{ from } q \text{ side}} \, \mathrm{d}S - \int_S \underbrace{\left(\mathbf{\Phi}^p + \rho_t^p \Psi^p (\mathbf{v}^p - \mathbf{u}^I)\right) \cdot \xi}_{\text{Flux of } \Psi \text{ from } p \text{ side}} \, \mathrm{d}S = \int_S \underbrace{\zeta^I}_{\text{Interfacial generation of } \Psi} \mathrm{d}S$$

- $\mathbf{u}^I$ Interface velocity
- $\mathbf{v}$ Mass-avg. velocity
- Ψ Quantity we are conserving
- Φ Non-convective (diffusive) flux



Note that if $\zeta^I = 0$

and $\mathbf{u}^I = 0$

then $\mathbf{n}_i^p \cdot \xi = \mathbf{n}_i^q \cdot \xi$

$\mathbf{u}^I$ may be related to ζ^I (e.g. ablation)

We would need a model for this.

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See T&K §1.3

Interfacial Balance Equations

$$\int_S \underbrace{\left(\mathbf{\Phi}^q + \rho_t^q \Psi^q (\mathbf{v}^q - \mathbf{u}^I)\right) \cdot \xi}_{\text{Flux of } \Psi \text{ from } q \text{ side}} \,\mathrm{dS} - \int_S \underbrace{\left(\mathbf{\Phi}^p - \rho_t^p \Psi^p (\mathbf{v}^p - \mathbf{u}^I)\right) \cdot \xi}_{\text{Flux of } \Psi \text{ from } p \text{ side}} \,\mathrm{dS} = \int_S \underbrace{\zeta^I}_{\text{Interfacial generation of } \Psi} \,\mathrm{dS}$$

	Continuity	Momentum	Energy	Species
Ψ	1	$\mathbf{v}$	$e_0 = u + \frac{1}{2}\mathbf{v}\cdot\mathbf{v}$	ω_i
$\mathbf{\Phi}$	0	$p\mathbf{I} + \tau$	$\mathbf{q} + (p\mathbf{I} + \tau)\cdot\mathbf{v}$	$\mathbf{j}_i$
ζ	0	$\sum_{i=1}^n \rho_i \mathbf{f}_i$	$\sum_{i=1}^n \rho_i \mathbf{f}_i \cdot \mathbf{u}_i$	σ_i
ζ^I	0	0	0	σ_i^I

“Bulk” Governing Equations

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho \mathbf{v}$$

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

$$\frac{\partial \rho \omega_i}{\partial t} = -\nabla \cdot (\rho \omega_i \mathbf{v}) - \nabla \cdot \mathbf{j}_i + s_i$$

$$\frac{\partial \rho e_0}{\partial t} = -\nabla \cdot (\rho e_0 \mathbf{v}) - \nabla \cdot \mathbf{q} - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) - \nabla \cdot (p\mathbf{v}) + \sum_{i=1}^{n_s} \mathbf{f}_i \cdot (\rho_i \mathbf{v} + \mathbf{j}_i)$$

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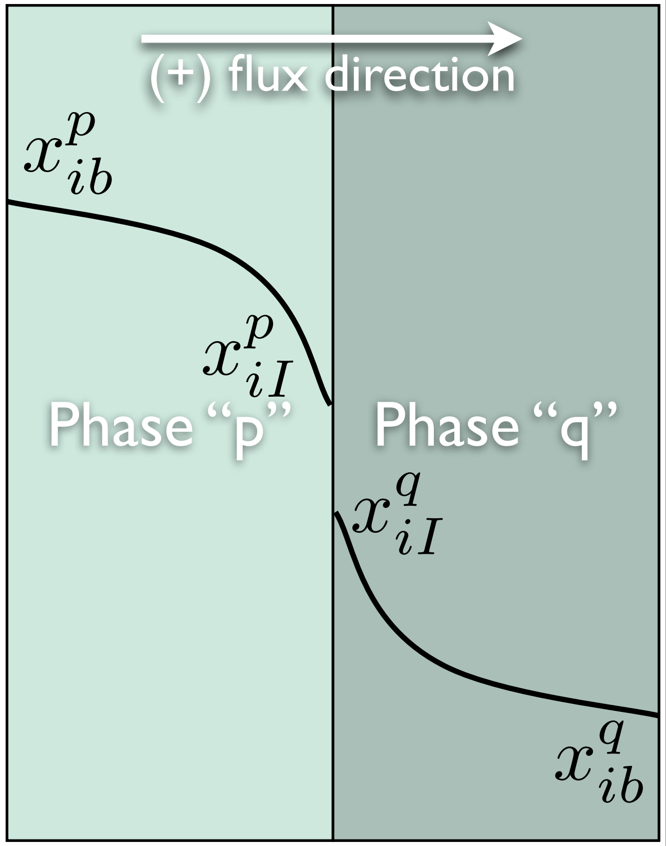
See T&K §7.1

Mass Transfer Coefficients

Solution Options:

- Resolve the spatial gradients, solve equations as we have thus far, with appropriate interface BCs (flux matching at interface)
- Model the diffusion process at a "larger" scale between interface and "bulk"



Discrete approximation to Fick's Law for diffusion normal to the interface:

$$(J^p) \approx -c_t^p[D^p]\frac{(x_I^p)-(x_b^p)}{L}$$

Note that if L is "big" then we may miss important features.

$$\begin{aligned}(J^p) &\approx c_t^p[D^p]\frac{(x_b^p)-(x_I^p)}{L}\\ \boxed{(J) \approx c_t[k_b^\bullet](\Delta x)}\end{aligned}$$

$$\begin{aligned}\Delta x_i^p &\equiv x_{ib}^p - x_{iI}^p\\ \Delta x_i^q &\equiv x_{iI}^q - x_{ib}^q\end{aligned}$$

Mass transfer coefficient

- Incorporates "boundary layer" thickness and D_{ij}.
- If L is "large," then we are really burying a lot of physics in D/L.
- Is a function of **J** itself!
- Must be corrected to account for the fact that we are burying more physics in this description.
- Often used for turbulent boundary layers also (more later)

"Low-flux" M.T. coefficient

$$[k_b^\bullet] = [k_b][\Xi_b]$$

More later (patience)

Correction Matrix

See T&K §7.1.3

Comparison w/ Fick's Law

Fick's Law

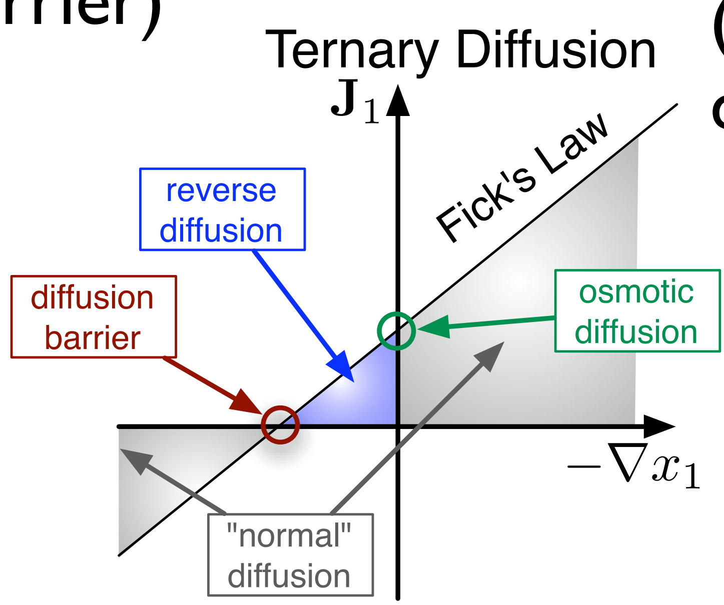
$$(\mathbf{J}) = -c_t[D](\nabla x)$$

- Fick's law can be derived from irreversible thermodynamics.
- $[D]$ are unique (for a given composition and ordering)
- Can describe multicomponent effects (osmotic diffusion, reverse diffusion, diffusion barrier)

M.T. Coeff Approach

$$(J) = c_t[k_b^\bullet](\Delta x)$$

- Empirical equation.
- $[k_b^\bullet]$ defined by (J) and (Δx). This means that there are n-1 equations defining a matrix with $(n\text{-}1)\times(n\text{-}1)$ elements. This implies that the $[k_b^\bullet]$ are *not unique*.
- Can describe multicomponent effects (osmotic diffusion, reverse diffusion, diffusion barrier)



See T&K §7.1.1

Binary Mass Transfer Coefficients

$$k_b = \frac{J_{1b}}{c_t \Delta x_1}$$ "Low-flux limit," binary system $$k_b = \lim_{N_1 \to 0} \frac{N_{1b} - x_{1b} N_t}{(x_{1b} - x_{1I})}$$ $$k_b^\bullet = k_b \Xi_b$$

This defines the low-flux MTC

$k_b \; [=] \; \mathrm{m/s}$ **Is it a velocity?**

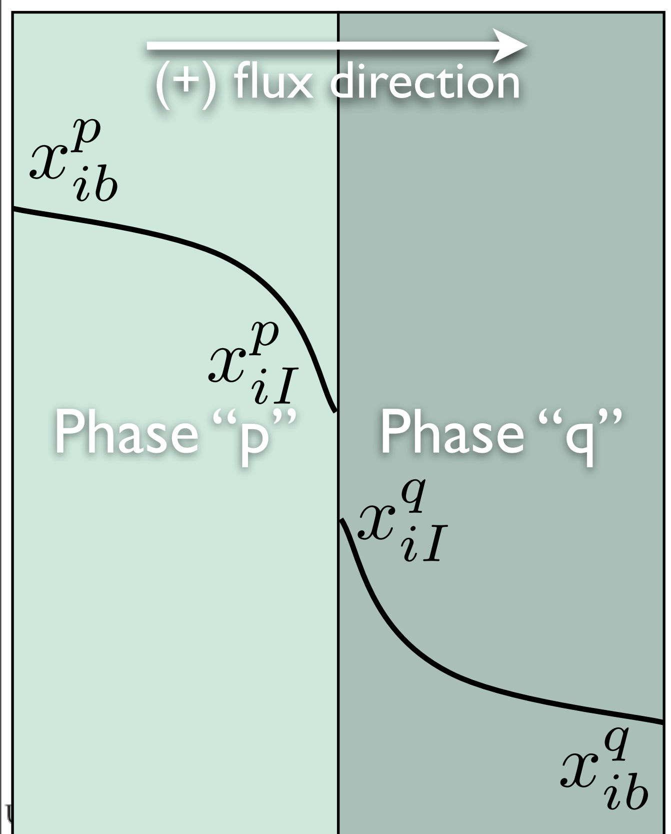
$$k_b = \frac{J_{1b}}{c_t \Delta x_1}, \qquad J_{1b} = c_t x_{1b}(u_1 - u)$$

$$k_b = \frac{(u_1 - u)}{\Delta x_1 / x_{1b}}$$

$$(u_1 - u) = \frac{k_b \Delta x_1}{x_{1b}}$$

For a binary system, $k_b>0$, and is maximized when $\Delta x_1=1$ (which also implies $x_{1b}=1$)

k_b - maximum velocity (relative to mixture velocity) at which a component can be transfered in a binary system.



Summary & a Path Forward

$$(J) = c_t[k_b^\bullet](\Delta x) \qquad [k_b^\bullet] = [k_b][\Xi_b]$$

- MTC Approach is useful when we don't want to resolve the diffusion path
  - Interfaces, boundary layers, turbulence, etc.
- Formulation is a true multicomponent formulation
  - Can describe osmotic diffusion, reverse diffusion, diffusion barrier.
- Still need to determine how to get $[k_b]$ and $[\Xi_b]$
  - $[k_b]$ cannot be uniquely determined by (J) and (Δx).
  - $[k_b]$ must be corrected ... how do we get $[\Xi_b]$?
  - We will return to this later:
    - Film theory (turbulent boundary layer theory)
    - Correlations (heat-transfer analogies)
- Can we get the total fluxes from (J)?
  - We will consider this issue soon. But first ... Film Theory!

See T&K Chapter 8

Film Theory

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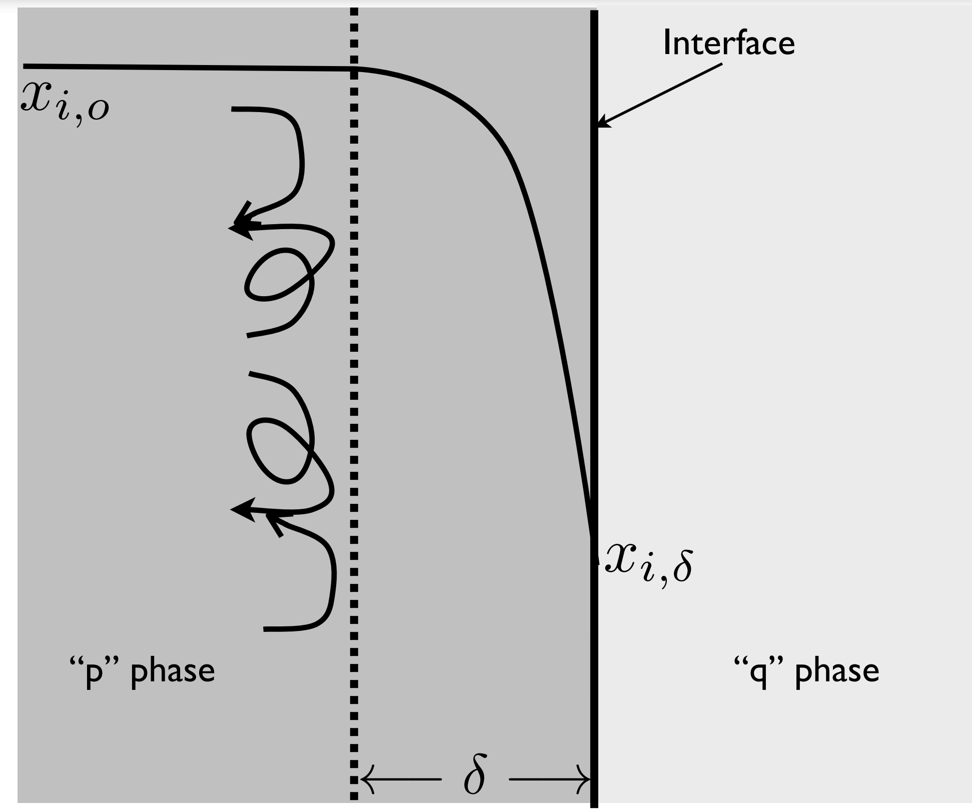
Perspective

$$(J) = c_t[k_b^\bullet](\Delta x) \qquad [k_b^\bullet] = [k_b][\Xi_b]$$

- We want to approximate J_i using Δx_i rather than resolving ∇x_i.
  - Need a way to get $[\Xi_b]$ and $[k_b]$.
  - *Film Theory* is one way to get $[\Xi_b]$ and $[k_b]$. It uses an *analytic solution* to the Maxwell-Stefan equations to deduce what $[\Xi_b]$ and $[k_b]$ should be.
- To get N_i:
  - Could solve governing equations (momentum) & fully resolve everything...
    - This defeats the purpose of using the MTC approach!
  - Use the "bootstrap" approach (inject specific knowledge of the problem to get N_i from J_i). More soon!

Formulation - Film Theory



Concepts:

- Mass transfer occurs in a thin "film" or boundary layer. Outside of this, the composition is uniform due to well-mixedness (e.g. turbulence).
- Gradients in the boundary-tangential direction are negligible compared to boundary-normal gradients.

Formulation:

- One-dimensional continuity and species at steady-state w/o reaction:

$$\nabla \cdot N_t = 0, \qquad \nabla \cdot N_i = 0$$
$$\Downarrow$$
$$N_t = const., \qquad N_i = const.$$

- Constitutive relations (*i.e.* expressions for J_i) given by either GMS or Fick's Law.
- Boundary conditions: known compositions

$$x_i = x_{i0} \qquad r = r_0$$
$$x_i = x_{i\delta} \qquad r = r_\delta.$$

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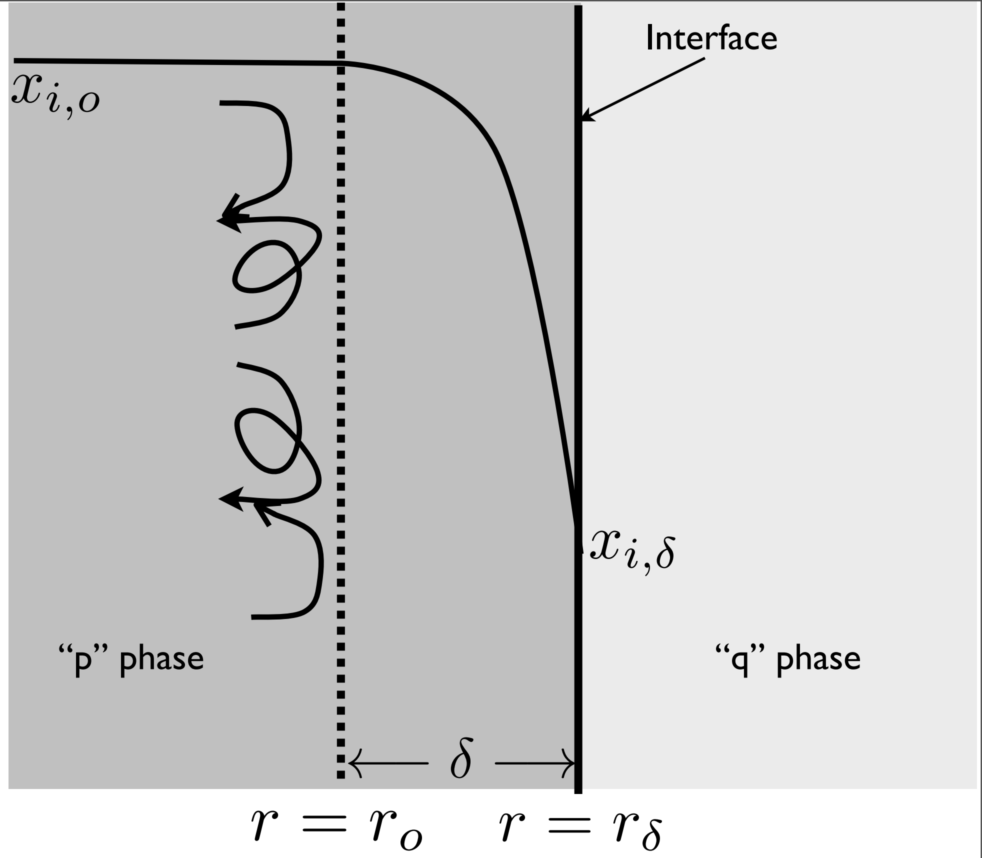
See T&K §8.3 & Appendix B

Assumptions:

- Steady-state
- 1-D
- No reaction
- Isothermal
- Ideal mixtures $[\Gamma]=[I]$.
- "small" pressure gradients
- uniform body forces



Normalized coordinate: $\eta \equiv \dfrac{r - r_0}{\ell}, \qquad \ell \equiv r_\delta - r_0$

GMS:
$$\frac{\mathrm{d}x_i}{\mathrm{d}r} = \sum_{j=1}^{n} \frac{(x_i N_j - x_j N_i)}{c_t Đ_{ij}}$$

GMS (n-1 dim) in terms of normalized coordinate.

$$\frac{\mathrm{d}x_i}{\mathrm{d}\eta} = \Phi_{ii}x_i + \sum_{\substack{j=1\\ j\neq i}}^{n-1} \Phi_{ij}x_j + \phi_i$$

$$\frac{\mathrm{d}(x)}{\mathrm{d}\eta} = [\Phi](x) + (\phi)$$

$$\Phi_{ii} = \frac{N_i}{c_t Đ_{in}/\ell} + \sum_{\substack{k=1\\ k\neq i}}^{n} \frac{N_k}{c_t Đ_{ik}/\ell},$$

$$\Phi_{ij} = -N_i\left(\frac{1}{c_t Đ_{ij}/\ell} - \frac{1}{c_t Đ_{in}/\ell}\right),$$

$$\phi_i = -\frac{N_i}{c_t Đ_{in}/\ell}$$

Analytic solution (assuming N_i are all constant)
see T&K Appendix B

$$(x - x_0) = \Big[\exp\,[[\Phi]\eta] - [I]\Big]\Big[\exp[\Phi] - [I]\Big]^{-1}(x_\delta - x_0)$$

Matrix exponential!
$\exp[\Phi] \neq [\exp(\Phi_{ij})]$!

Given the total fluxes (to get Φ), we can obtain the compositions analytically!

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$$(x - x_0) = \Big[\exp\left[[\Phi]\eta\right] - [I]\Big]\Big[\exp[\Phi] - [I]\Big]^{-1}(x_\delta - x_0)$$

From the solution, we can calculate the diffusive fluxes and use them to help us determine what the MTCs are for this problem.

Fick's Law: $$(J) = -c_t[D]\frac{\mathrm{d}(x)}{\mathrm{d}r}$$

$$(J) = -\frac{c_t}{\ell}[D]\frac{\mathrm{d}(x)}{\mathrm{d}\eta} = c_t[k_b^\bullet](\Delta x)$$

MTC Formulation: $(J) = c_t[k_b^\bullet](\Delta x)$ $\qquad [k_b^\bullet] = [k_b][\Xi_b]$

$$\frac{\mathrm{d}(x)}{\mathrm{d}\eta} = [\Phi]\left[\exp[[\Phi]\eta]\left[\exp[\Phi] - [I]\right]^{-1}(x_\delta - x_0)\right.$$

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$$\frac{\mathrm{d}(x)}{\mathrm{d}\eta} = [\Phi]\left[\exp[[\Phi]\eta]\left[\exp[\Phi] - [I]\right]^{-1}(x_\delta - x_0)\right]$$

At η=0

$$(J_0) = \tfrac{c_t}{\ell}[D_0][\Phi]\left[\exp[\Phi] - [I]\right]^{-1}(x_0 - x_\delta)$$

$$[k_0^\bullet] = \tfrac{1}{\ell}[D_0][\Phi]\left[\exp[\Phi] - [I]\right]^{-1}$$

Low-flux limit:

$$k_b = \lim_{N_1 \to 0} \frac{N_{1b} - x_{1b}N_t}{(x_{1b} - x_{1I})} = \frac{J_{1b}}{c_t \Delta x_1}$$

$$[k_0] = \tfrac{1}{\ell}[D_0]$$

Correction matrix:

$$[\Xi_0] = [\Phi]\left[\exp[\Phi] - [I]\right]^{-1}$$

At η=1

$$(J_\delta) = \tfrac{c_t}{\ell}[D_\delta][\Phi]\left[\exp[\Phi]\right]\left[\exp[\Phi] - [I]\right]^{-1}(x_0 - x_\delta)$$

$$[k_\delta] = \tfrac{1}{\ell}[D_\delta]$$

$$[\Xi_\delta] = [\Phi]\exp[\Phi]\left[\exp[\Phi] - [I]\right]^{-1} = [\Xi_0]\exp[\Phi]$$

Re-Cap

- We can now easily solve for (x) given (N).
  - Assumes (N) is constant.
- We can also easily solve for (J) directly given (N).
- We must specify:
  - $[\Phi]$, which is a function of (x), (N), $Đ_{ij}$ and ℓ.
  - $[k]$, the low-flux MTC matrix.
  - $[\Xi]$ - the correction factor matrix.
- Coming soon: solution procedure

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See T&K §8.3.1

Calculating [k]

$$[k] = \frac{1}{\ell}[D]$$

$$\begin{aligned} R_{ii} &= \frac{x_i}{\kappa_{in}} + \sum_{\substack{k=1\\k\neq i}}^{n} \frac{x_k}{\kappa_{ik}}, \\ R_{ij} &= -x_i \left(\frac{1}{\kappa_{ij}} - \frac{1}{\kappa_{in}} \right), \\ \kappa_{ij} &\equiv \frac{Đ_{ij}}{\ell} \end{aligned}$$

Binary low-flux limit MTC

← compare →

$$\begin{aligned} B_{ii} &= \frac{x_i}{Đ_{in}} + \sum_{j\neq i}^{n} \frac{x_j}{Đ_{ij}}, \\ B_{ij} &= -x_i \left(\frac{1}{Đ_{ij}} - \frac{1}{Đ_{in}} \right) \end{aligned}$$

$$[k] = [R]^{-1}$$

$$[k] = \frac{1}{\ell}[B]^{-1}$$

Notes

- We have a routine to calculate $[B]$ given (x) and $[Đ]$. We can re-use this to get $[R]$ by passing in (x) and $[\kappa]$.
- Alternatively, just calculate $[B]^{-1}$ and then scale by ℓ.

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See T&K §8.3.3 & Appendix A

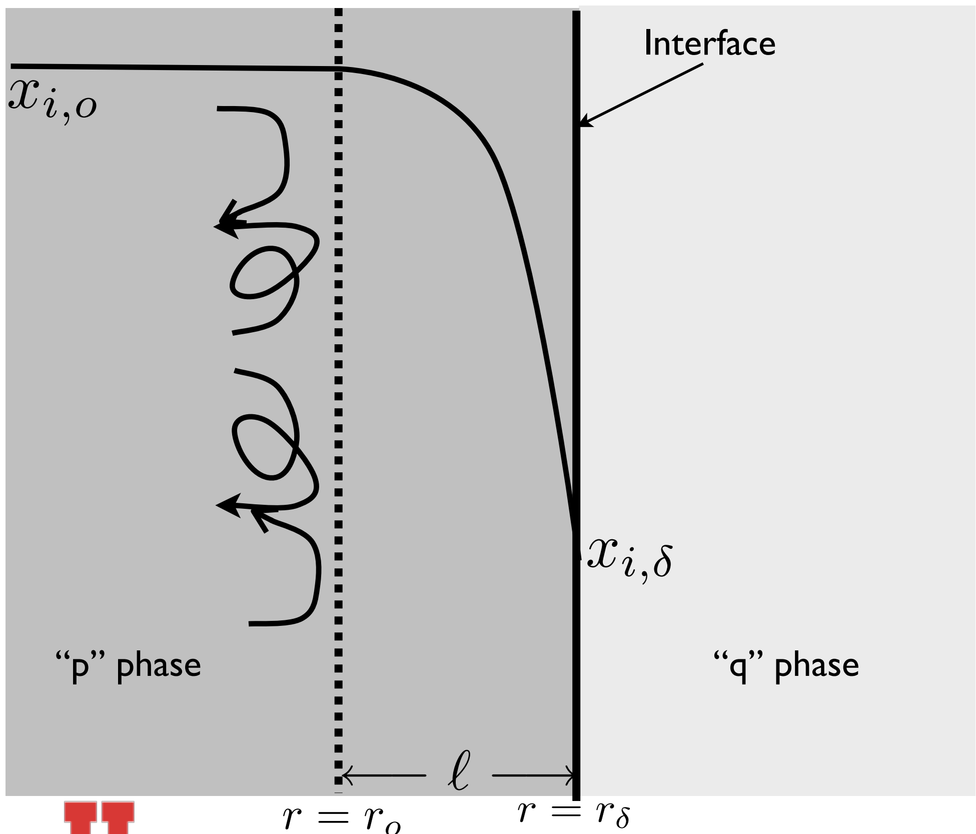
Calculating $[\Xi]$

Recall what we found for $[\Xi]$ from film theory:

At $r = r_0$ (η=0) $\quad [\Xi_0] = [\Phi]\left[\exp[\Phi] - [I]\right]^{-1}$

At $r = r_\delta$ (η=1) $\quad [\Xi_\delta] = [\Phi]\exp[\Phi]\left[\exp[\Phi] - [I]\right]^{-1} = [\Xi_0]\exp[\Phi]$

recall: $\exp[\Phi]$ is a matrix exponential;
$\exp[\Phi] \neq [\exp(\Phi_{ij})]$!



$$[\Xi] = \sum_{i=1}^{n} \hat{\Xi}_i \left\{ \frac{\prod_{\substack{j=1\\ j\neq i}}^{m} \left[[\Phi] - \hat{\Phi}_j [I]\right]}{\prod_{\substack{j=1\\ j\neq i}}^{m} \left[\hat{\Phi}_i - \hat{\Phi}_j [I]\right]} \right\}$$

$$\hat{\Xi}_{i0} = \frac{\hat{\Phi}_i}{\exp\hat{\Phi}_i - 1} \qquad \hat{\Xi}_{i\delta} = \frac{\hat{\Phi}_i \exp\hat{\Phi}_i}{\exp\hat{\Phi}_i - 1}$$

m - number of eigenvalues of Φ

OR, see "**expm**" function in MATLAB.

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Shortcuts...

Re-use the `B_matrix.m` code by passing different arguments!

$$
\begin{aligned}
B_{ii} &= \frac{x_i}{Đ_{in}} + \sum_{j\neq i}^{n} \frac{x_j}{Đ_{ij}}, \\
B_{ij} &= -x_i \left(\frac{1}{Đ_{ij}} - \frac{1}{Đ_{in}} \right)
\end{aligned}
\quad \Longrightarrow \quad
\boxed{
\begin{aligned}
B_{ii} &= \frac{\alpha_i}{\beta_{in}} + \sum_{j\neq i}^{n} \frac{\alpha_j}{\beta_{ij}}, \\
B_{ij} &= -\alpha_i \left(\frac{1}{\beta_{ij}} - \frac{1}{\beta_{in}} \right)
\end{aligned}
}
$$

$$
\begin{aligned}
\alpha_i &= x_i \\
\beta_{ij} &= Đ_{ij}
\end{aligned}
$$

$$
\begin{aligned}
\Phi_{ii} &= \frac{N_i}{c_t Đ_{in}/\ell} + \sum_{\substack{k=1\\k\neq i}}^{n} \frac{N_k}{c_t Đ_{ik}/\ell}, \\
\Phi_{ij} &= -N_i \left(\frac{1}{c_t Đ_{ij}/\ell} - \frac{1}{c_t Đ_{in}/\ell} \right)
\end{aligned}
$$

$$
\begin{aligned}
\alpha_i &= N_i \\
\beta_{ij} &= \frac{c_t}{\ell} Đ_{ij}
\end{aligned}
$$

$$
\begin{aligned}
R_{ii} &= \frac{x_i}{\kappa_{in}} + \sum_{\substack{k=1\\k\neq i}}^{n} \frac{x_k}{\kappa_{ik}}, \\
R_{ij} &= -x_i \left(\frac{1}{\kappa_{ij}} - \frac{1}{\kappa_{in}} \right), \\
\kappa_{ij} &\equiv \frac{Đ_{ij}}{\ell}
\end{aligned}
$$

$$
[k] = [R]^{-1}
$$

$$
\begin{aligned}
\alpha_i &= x_i \\
\beta_{ij} &= \frac{1}{\ell} Đ_{ij}
\end{aligned}
$$

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The "Bootstrap" Problem

Getting N_i from J_i and Physical Insight

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See T&K §7.2

The "Bootstrap" Problem

If we know the diffusive fluxes, can we obtain the total fluxes?

$$J_i \xrightarrow[\text{Problem}]{\text{Bootstrap}} N_i$$

Can be solved for some special cases.

General problem formulation: $$\sum_{i=1}^{n} \nu_i N_i = 0$$

ν_i are *determinacy coefficients* (values depend on the specific case/assumptions)

Species Molar Flux:
$$\begin{aligned} N_i &= J_i + x_i N_t \\ \nu_i N_i &= \nu_i J_i + \nu_i x_i N_t \\ \sum_{i=1}^{n} \nu_i N_i &= \sum_{i=1}^{n} \nu_i J_i + N_t \sum_{i=1}^{n} \nu_i x_i = 0 \end{aligned}$$

Solve for N_t:
$$N_t = -\left(\sum_{i=1}^{n} \nu_i J_i\right)\left(\sum_{i=1}^{n} \nu_i x_i\right)^{-1}$$

remove the n^{th} diffusive flux:
$$N_t = -\sum_{k=1}^{n-1} \underbrace{\frac{\nu_k - \nu_n}{\sum_{j=1}^{n} \nu_j x_j}}_{\Lambda_k} J_k$$

$$\begin{aligned} N_i &= J_i + x_i N_t \\ &= J_i - x_i \sum_{k=1}^{n-1} \Lambda_k J_k \end{aligned}$$

$$N_i = \sum_{k=1}^{n-1} \beta_{ik} J_k$$

$$\beta_{ik} \equiv \delta_{ik} - x_i \Lambda_k$$

If we can get β_{ik} (or Λ_k), we can solve the problem!

See T&K §7.2

Solving the Bootstrap Problem

$$\sum_{i=1}^{n} \nu_i N_i = 0 \qquad N_i = \sum_{k=1}^{n-1} \beta_{ik} J_k \qquad \beta_{ik} \equiv \delta_{ik} - x_i \Lambda_k \qquad \Lambda_k = (\nu_k - \nu_n)\left(\sum_{j=1}^{n} \nu_j x_j\right)^{-1}$$

Bootstrap matrix

Equimolar counterdiffusion: $N_t = 0$

- Isobaric, closed systems...

$$N_i = J_i \implies \nu_i = \nu_n, \quad i = 1, 2, \ldots, n$$

$$\boxed{\beta_{ik} = \delta_{ik}}$$

Stefan Diffusion: $N_n = 0$

One component has a zero flux, N_n=0.

- Condensation/evaporation
- Absorption (similar to condensation)

$$\nu_i = 0, \quad \nu_n \neq 0, \quad (N_n = 0)$$

$$\boxed{\beta_{ik} = \delta_{ik} + \frac{x_i}{x_n}}$$

Flux ratios specified: $N_i = z_i N_t$

- Condensation of mixtures (T&K Ch. 15)
- Chemical reaction where the chemistry is fast relative to the diffusion (diffusion-controlled).

$$\begin{aligned} N_i &= x_i N_t + J_i \\ N_i &= x_i \frac{N_i}{z_i} + J_i \end{aligned}$$

$$\sum_{i=1}^{n} N_i \left(1 - \frac{x_i}{z_i}\right) = \sum_{i=1}^{n} J_i = 0$$

$$\sum_{i=1}^{n} \nu_i N_i = 0 \;\Rightarrow\; \nu_i = 1 - \frac{x_i}{z_i}$$

$$\boxed{\beta_{ik} = \frac{\delta_{ik}}{1 - x_i/z_i}}$$

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Using the Boostrap Matrix

$$N_i = \sum_{k=1}^{n-1} \beta_{ik} J_k$$

Write this in matrix form:
$$\begin{aligned} N_t &= -(\Lambda)^T (J) \\ (N) &= [\beta](J) \end{aligned}$$

Use with MTCs:

In the "bulk:"

$$\begin{aligned} (J_b) &= c_{t,b}[k_b^\bullet](\Delta x_b) \\ (N_b) &= [\beta_b](J_b) = c_{t,b}[\beta_b][k_b^\bullet](\Delta x_b) \end{aligned}$$

At the interface:

$$\begin{aligned} (J_I) &= c_{t,I}[k_I^\bullet](\Delta x_I) \\ (N_I) &= [\beta_I](J_I) = c_{t,I}[\beta_I][k_I^\bullet](\Delta x_I) \end{aligned}$$

$(N_I) = (N_b)$ (no reaction in boundary layer)

Binary System

$$\begin{aligned} N_1 = c_t \beta_I k_I^\bullet \Delta x_1 &= c_t \beta_b k_b^\bullet \Delta x_1 \\ &\Downarrow \\ \beta_I k_I^\bullet &= \beta_b k_b^\bullet = \frac{N_1}{c_t \Delta x_1} \end{aligned}$$

Multicomponent System

$$[\beta_I][k_I^\bullet](\Delta x) = [\beta_b][k_b^\bullet](\Delta x)$$

Since $[A](x)=[B](x)$ doesn't imply that $[A]=[B]$, we cannot conclude anything about the relationship between $[\beta_b][k_b^\bullet]$ and $[\beta_I][k_I^\bullet]$.

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Re-Cap

- Bootstrap problem: exists because we don't want to solve all of the governing equations, but we want to get the total fluxes anyway.
- Interphase mass transfer: simplified approach to avoid fully resolving interfaces.
    - Non-uniqueness of MTCs

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See T&K §8.3.3

Film Theory: A "Simple" Solution Procedure

Given (x_0), (x_δ), c_t, κ_{ij},

1. Compute $[k]=[D]/\ell$.
2. Compute $[\beta]$ from the appropriate expressions given the specific problem.
3. Estimate $(N)=c_t[\beta][k](\Delta x)$. (This does not employ the correction matrix since we don't yet have $[\Xi]$).
4. Calculate $[\Phi]$
5. Calculate $[\Xi]$
6. Calculate $(J)=c_t[k][\Xi](\Delta x)$.
7. Calculate $(N)=[\beta](J)$.
8. Check for convergence on (N). If not converged, return to step 4.

$$\begin{aligned}
\Phi_{ii} &= \frac{N_i}{c_t Đ_{in}/\ell} + \sum_{\substack{k=1\\k\neq i}}^{n} \frac{N_k}{c_t Đ_{ik}/\ell}, \\
\Phi_{ij} &= -N_i\left(\frac{1}{c_t Đ_{ij}/\ell} - \frac{1}{c_t Đ_{in}/\ell}\right)
\end{aligned}$$

Uses successive substitution to converge (N). This could lead to poor convergence (or no convergence) depending on the guess for (N).

<u>Note</u>: we could use "better" ways to iterate (N) to improve convergence.

See Algorithms 8.2 & 8.3 in T&K (pp. 180, 182)

See T&K §8.7

Nonideal Systems

Recall we assumed $[\Gamma]=[I]$. What if that is not valid???

Approach:

- Repeat original analysis, retaining $[\Gamma]$.
- Write $[D]=[\Gamma][B]^{-1}$.
- We can re-use the original results directly, using $[D]=[\Gamma][B]^{-1}$... (typically also approximate $[\Gamma]$ as constant)
- See also T&K §8.7.2, §8.8.4

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See T&K §8.8

Estimation of MTCs [k]

Motivation:

- Prior approaches have required knowledge of ℓ . What if we don't know this? (often the case)
- Idea: use correlations (dimensionless groups)

Sherwood number: $$[\mathrm{Sh}] = d[k][D]^{-1}$$ often correlated as function of Re, $[\mathrm{Sc}]$.

Stanton number: $$[\mathrm{St}] = [k]/u$$ often correlated as function of $[\mathrm{Sc}]$.

$[\mathrm{Sc}]=\nu[D]^{-1}$

These typically correlate the low-flux MTCs. Sill need to apply $[\Xi]$.

Correlations abound! Be sure that the one you use is appropriate!

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