Linearized Theory

CHEN 6603

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Motivation

What assumptions?

Fick's Second Law (molar form):

$$\frac{\partial (x)}{\partial t} + \nabla \cdot \mathbf{u}(x) = [D](\nabla^2 x)$$

- Fick's 2nd law is useful, but is still coupled due to the diffusion coefficient matrix.
  - Under some additional assumptions (see equimolar counterdiffusion example), the equations decouple.
- We would like to be able to solve transient problems while maintaining the coupling between equations.
  - Linearized theory let's us do this.

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Linearized Theory Formulation

Eigenvalue decomposition of $[D]$: $$[P]^{-1}[D][P] = [\hat{D}]$$

Columns of $[P]$ are the eigenvectors of $[D]$

Diagonal matrix, entries are eigenvalues of $[D]$.

Fick's 2nd Law: $$\frac{\partial(x)}{\partial t} = -\nabla\cdot(\mathbf{u}(x)) + [D](\nabla^2 x)$$

Assumes $[P]$ is constant!

$$\frac{\partial \overbrace{[P]^{-1}(x)}^{(\hat{x})}}{\partial t} = -\nabla\cdot(\mathbf{u}\overbrace{[P]^{-1}(x)}^{(\hat{x})}) + \overbrace{[P]^{-1}[D][P]}^{[\hat{D}]}\overbrace{[P]^{-1}(\nabla^2 x)}^{(\nabla^2\hat{x})},$$

$[P][P]^{-1} = [I]$

$$\frac{\partial(\hat{x})}{\partial t} = -\nabla\cdot(\mathbf{u}(\hat{x})) + [\hat{D}](\nabla^2\hat{x}).$$

Decoupled set of equations, since $[\hat{D}]$ is diagonal.

Approach:

- Transform the problem
- Solve the transformed problem
- transform the results back

Terminology

$$\frac{\partial(\hat{x})}{\partial t} = -\nabla \cdot (\mathbf{u}(\hat{x})) + [\hat{D}](\nabla^2 \hat{x})$$

$(\hat{x})$ Pseudo compositions $(\hat{x}) = [P]^{-1}(x)$

$[\hat{D}]$ Pseudo diffusivity $[P]^{-1}[D][P] = [\hat{D}]$

$[P]$ Modal matrix
(columns are eigenvalues of $[D]$).

Diffusion Fluxes

If needed, the diffusive fluxes may be post-processed.

$$
\begin{aligned}
(\mathbf{J}) &= -c_t [D](\nabla x), \\
[P]^{-1}(\mathbf{J}) &= -c_t [P]^{-1}[D][P][P]^{-1}(\nabla x) \\
(\hat{\mathbf{J}}) &= -c_t [\hat{D}](\nabla \hat{x})
\end{aligned}
$$

$$
(\hat{\mathbf{J}}) = [P]^{-1}(\mathbf{J}), \quad (\mathbf{J}) = [P](\hat{\mathbf{J}})
$$

Notes:

- $(\mathbf{J})$ should be computed using the same approximations that went into the original equation set that was used to obtain (x).

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Algorithm

1. Obtain the Fickian diffusion matrix $[D]$ at some representative composition, temperature and pressure.
2. Calculate the modal matrix $[P]$ and its inverse $[P]^{-1}$.
3. Calculate the initial/boundary conditions in pseudo-composition space: $(\hat{x}) = [P]^{-1}(x)$
4. Calculate the diagonal $[\hat{D}]$ matrix (pseudo-diffusivity matrix) via $[\hat{D}] = [P]^{-1}[D][P]$
5. Obtain the solution for each species in pseudo-composition space by solving the $(n\text{-}1)$ independent PDEs.
6. Convert back to real compositions via the transformation
$$(x) = [P](\hat{x})$$

NOTE: the Matlab "eig" function will calculate the $[P]$ and $[\hat{D}]$ matrices for you!

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Re-Cap

- $[\hat{D}]$ is the same for all reference frames (T&K §3.2.2)
- Assumes that $[D]$ is constant.
- No thermal diffusion (Soret effect)
- Body forces act uniformly on all species (e.g. gravity)
- Negligible pressure gradient (to eliminate pressure gradient from driving force in Fick's law)
- c_t = constant
- Could be solved in mass form as well, with analogous assumptions (may be more restrictive).

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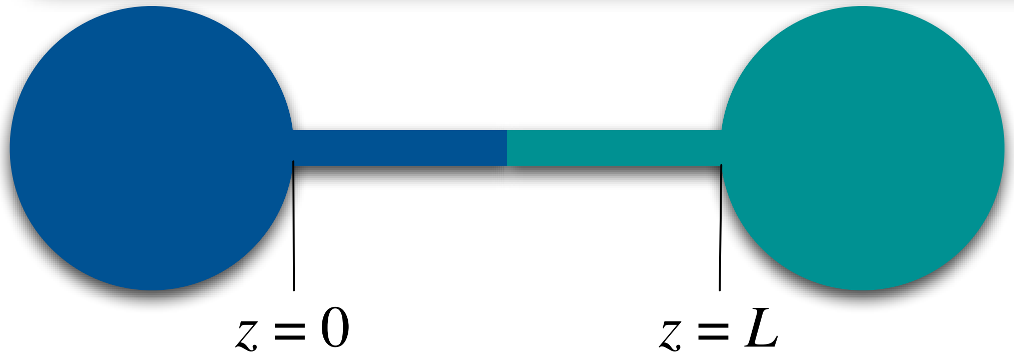
T&K §5.4

Example: 2 Bulb Problem (again)



$$\begin{aligned} x_i &= x_{i0} \qquad z = 0, \\ x_i &= x_{iL} \qquad z = L, \end{aligned}$$

$$\begin{aligned} \frac{\mathrm{d}(x^0)}{\mathrm{d}t} &= \frac{A}{LV_0}\left(1+\frac{V_0}{V_L}\right)[D]\left((x^\infty)-(x^0)\right) \\ &= \beta[D]\left((x^\infty)-(x^0)\right), \end{aligned}$$

$$\beta \equiv \frac{A}{LV_0}\left(1+\frac{V_0}{V_L}\right)$$

Constant for a given geometry.

Must solve this (coupled) system of ODEs for the change in the composition in bulb 0 in time.

Linearized theory lets us easily solve this system without decoupling the physics.

$$\frac{\mathrm{d}(\hat{x}^0)}{\mathrm{d}t} = \beta[\hat{D}]\left((\hat{x}^\infty)-(\hat{x}^0)\right),$$

$$\frac{\hat{x}_i^0 - \hat{x}_i^\infty}{\hat{x}_i^{0,o} - \hat{x}_i^\infty} = \exp\left(-\beta\hat{D}_i(t-t_o)\right)$$

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