Lecture 22: Multicomponent Equations & Free Convection

* Now that we have been through the multicomponent mass balances, what (if anything) needs to be done for our momentum and energy balances?

I. Equations of change for multicomponent systems

* mass

(species continuity)

$$\rho \frac{D\omega_\alpha}{Dt} = \nabla \cdot \left[\sum_{\beta=1}^{N_s} \rho D_{\alpha\beta} \nabla \omega_\beta \right] + r_\alpha$$

(total continuity)

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \underline{v})$$

* momentum

$$\rho \frac{D\underline{v}}{Dt} = -\nabla p + \mu \nabla^2 \underline{v} + \left(\frac{\mu}{3} + k \right) \nabla (\nabla \cdot \underline{v}) + \rho \underline{g}$$

- momentum is the same! It is unaffected by the multicomponent nature of the fluid.

* energy

- The energy equation has some significant modifications for muticomponent systems.

- The heat flux: $\underline{q} = -k \nabla T$ (single component)

gets an additional term: $\underline{q} = -k \nabla T + \sum_{\alpha=1}^{N_c} \frac{\overline{H}_\alpha}{M_\alpha} \underline{j}_\alpha$

This term is due to the enthalpy of different species that diffuse across the boundary.

$\bar{H}_\alpha$: partial molar enthalpy of species α

M_α: molecular weight of species α

$\underline{j}_\alpha$: diffusive flux of species α

- The enthalpy change from chemical reactions:

$$\sum_\alpha \bar{H}_\alpha R_\alpha$$

$\bar{H}_\alpha$: partial molar ethalpy of α

R_α: (molar) reaction

- The specific enthalpy $\hat{H}$ needs to account for the energy of mixing & formation.

- This all gets quite detailed & is not worth our time, since we are not focusing on this.

- This can be written as: (Eq. F in table 19.2-4)

specific volume

$$\rho \hat{C}_p \frac{DT}{Dt} = -\underline{\nabla}\cdot \underline{q} - \underline{\underline{\tau}} : \underline{\nabla}\underline{v} + \left(\frac{\partial \ln \hat{V}}{\partial \ln T}\right)_{p, x_A} \frac{Dp}{Dt} + \sum_{\alpha=1}^{N} \bar{H}_\alpha \left[\underline{\nabla}\cdot \underline{J}_\alpha - R_\alpha \right]$$

$\underline{q} = -k\underline{\nabla}T + \sum_\alpha \bar{H}_\alpha \underline{J}_\alpha$

$\mu \Phi_v + \kappa \Psi_v$ for Newtonian

$\underline{J}_\alpha$: molar flux of α w.r.t. mass velocity

$\underline{J}_\alpha = c_\alpha (\underline{v}_\alpha - \underline{v})$

* See Tables 19.2-2, 19.2-3, 19.2-4 for a complete summary. Also need all thermo info: $p = p(\rho, T, x_\alpha)$! $\hat{u} = \hat{u}(\rho, T, x_\alpha)$

* This is very general. Solids, liquids, gases. Multicomponent. compressible / incompressible, whatever you want! As a matter of fact, it is so general, it is only useful as a summary. Don't ever start here. You need to know what equations are good in what circumstance & use them when appropriate.

II. The Boussinesq Approximation

* In addition to assuming Fourier's law, Fick's law & Newton's law of viscosity, it is very useful to assume incompressibility. This really does simplify our equations a lot. However, temperature & concentration differences very easily lead to density differences. Is there another way to treat these kinds of flows w/o resorting to the mess above?

* Let's write our equation of state as:

$$\rho = \bar{\rho} + \left.\frac{\partial \rho}{\partial T}\right|_{\bar{T},\bar{\omega}_A} (T - \bar{T}) + \left.\frac{\partial \rho}{\partial \omega_A}\right|_{\bar{\rho},\bar{\omega}_A} (\omega_A - \bar{\omega}_A) + \ldots$$

- Taylor expansion about average T & average ω_A
  $\bar{\rho}$: avg density, $\bar{T}$: avg temp, $\bar{\omega}_A$: avg ω_A

- Expansion for a binary system only. Can add more terms, i.e. $\partial\rho/\partial\omega_B \cdot (\omega_B - \bar{\omega}_B)$ if needed.

- recall that

$$\beta = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P \quad : \text{ Isobaric thermal expansion coefficient}$$

$$\zeta = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial \omega_A}\right) \quad : \text{ solutal expansion coefficient}$$

$$\rho = \bar{\rho} - \bar{\rho}\bar{\beta}(T - \bar{T}) - \bar{\rho}\bar{\zeta}(\omega_A - \bar{\omega}_A)$$

- This is not silly, $\bar{\beta} \approx$ const for many liquids.

* Now, if we let $\rho = \bar{\rho}$ for all cases except the buoyancy term in the equation of motion, we get a pretty reasonable set of equations. This is called the <u>Boussinesq approximation</u>.

* For a <u>non-reacting</u>, <u>binary</u> system w/ const α & $\rho \mathcal{D}_{AB}$, this gives:

$\alpha = k/\rho\tilde{C}_p$

$$\boxed{\begin{aligned} &\rho \frac{D\underline{v}}{Dt} = -\underline{\nabla}\mathcal{P} + \mu\nabla^2\underline{v} - \left[\bar{\rho}\bar{\beta}(T-\bar{T}) + \bar{\rho}\bar{\xi}(\omega_A - \bar{\omega}_A)\right]\underline{g} \\ &\frac{DT}{Dt} = \alpha\nabla^2 T \qquad \underline{\nabla}\mathcal{P} = \nabla p - \bar{\rho}\underline{g} \\ &\frac{D\omega_A}{Dt} = \mathcal{D}_{AB}\nabla^2\omega_A \ , \qquad \underline{\nabla}\cdot\underline{v} = 0 \end{aligned}}$$

* Comments:

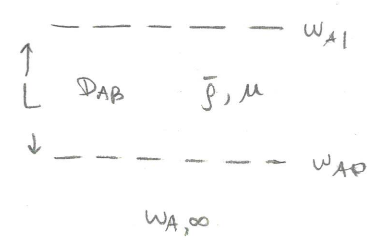
  - Assumes: Fourier's law, Fick's law, Newtonian Fluid.
    Binary, non-reacting, constant k, $\tilde{C}_p$, $\mathcal{D}_{AB}$
    Boussinesq.

  - Still very useful! Good for almost all simple liquids. Many gases. Can simplify for solids.
    Can relatively easily generalize for multicomponent or to include reactions.

  - <u>Much</u> better than doing fully compressible case.

III. Dimensional Analysis of Boussinesq Approximation

* There is much that can be done here. Let's just examine the case with a conc. difference for now:



A: solute
B: solvent

$w_{A1} > w_{A0}$
(backwards, so $\rho_1 > \rho_0$ ∴ density drives flow)

$$\rho \frac{D\underline{v}}{Dt} = -\underline{\nabla} \mathcal{P} + \mu \nabla^2 \underline{v} - \bar{\rho}\underline{g}\,\bar{\zeta}\,(w_A - \bar{w}_A)$$

$$\frac{D w_A}{Dt} = D_{AB} \nabla^2 w_A$$

* let length: L

time: "momentum diffusion" time scale L^2/ν

pressure: "ρu^2" $\Rightarrow$ $\bar{\rho}\left(\frac{\nu}{L}\right)^2 = \frac{\mu^2}{\bar{\rho} L}$ (not unique choice)

note: $\bar{\zeta}$ is dimensionless

$$\zeta = \frac{1}{\rho}\frac{\partial \rho}{\partial w_A}$$

* variables:

$\tilde{\underline{v}} = \underline{v}/(\nu/L)$ $\quad \tilde{x} = x/L$, $\tilde{\underline{g}} = \underline{g}/g$ (Because can)

$\tilde{t} = t/(L^2/\nu)$ $\quad \tilde{\nabla} = L\nabla$

$\tilde{\mathcal{P}} = \mathcal{P}/\bar{\rho}\left(\frac{\nu}{L}\right)^2$ $\quad \tilde{w}_A = \dfrac{w_A - w_{A0}}{\underbrace{w_{A1} - w_{A0}}_{\Delta w_A}}$ (∴ $\tilde{\bar{w}}_A$)

$$\frac{\bar{\rho}\,\nu}{L}\frac{\nu}{L^2}\frac{D\tilde{\underline{v}}}{D\tilde{t}} = -\frac{\bar{\rho}\,\nu^2}{L\,L^2}\tilde{\underline{\nabla}}\mathcal{P} + \frac{\mu\,\nu/L}{L^2}\tilde{\nabla}^2\tilde{\underline{v}}$$

$$- \bar{\rho} g\,\tilde{\underline{g}}\,\bar{\zeta}\,\Delta w_A\,(\tilde{w}_A - \tilde{\bar{w}}_A)$$

$$\nu\frac{\Delta w_A}{L^2}\frac{D\tilde{w}_A}{D\tilde{t}} = D_{AB}\frac{\Delta w_A}{L^2}\tilde{\nabla}^2\tilde{w}_A$$

$$\begin{cases} \dfrac{D\tilde{v}}{D\tilde{t}} = -\tilde{\nabla}\mathcal{P} + \dfrac{\cancel{L^3}}{\cancel{\bar{\rho}}\,\nu^2} \cdot \dfrac{\cancel{\mu}\,\nu}{\cancel{L^3}} \tilde{\nabla}^2\tilde{v} - \dfrac{\cancel{\bar{\rho}}\, g\,\Delta\omega_A L^3}{\cancel{\bar{\rho}}\,\nu^2} \tilde{g}\,\bar{\xi}\,(\tilde{\omega}_A - \tilde{\bar{\omega}}_A) \\[2ex] \dfrac{D\tilde{\omega}_A}{Dt} = \dfrac{D_{AB}\,\cancel{\Delta\omega_A}}{\cancel{L^2}} \dfrac{\cancel{L^2}}{\nu\,\cancel{\Delta\omega_A}} \tilde{\nabla}\tilde{\omega}_A \end{cases}$$

$$\frac{D\tilde{v}}{D\tilde{t}} = -\tilde{\nabla}\mathcal{P} + \tilde{\nabla}^2\tilde{v} - \underbrace{\frac{g\bar{\xi}(\omega_{A1}-\omega_{A0})L^3}{\nu^2}}\,\tilde{g}\,(\tilde{\omega}_A - \tilde{\bar{\omega}}_A)$$

$$\boxed{Gr = \frac{g\bar{\xi}(\omega_{A1}-\omega_{A0})L^3}{\nu}}$$

Grashoft # (masstransfer)

$$Gr = \frac{\text{buoyancy}}{\text{viscous forces}}$$

$$\frac{D\tilde{\omega}_A}{Dt} = \underbrace{\frac{D_{AB}}{\nu}}_{1/Sc} \tilde{\nabla}^2\tilde{\omega}_A \qquad \boxed{Sc = \frac{\nu}{D_{AB}}}$$

Schmidt #.

$$\boxed{\frac{D\tilde{v}}{D\tilde{t}} = -\tilde{\nabla}\mathcal{P} + \tilde{\nabla}^2\tilde{v} - Gr\,\tilde{g}\,(\tilde{\omega}_A - \tilde{\bar{\omega}}_A)}$$

$$\boxed{\frac{D\tilde{\omega}_A}{D\tilde{t}} = \frac{1}{Sc}\tilde{\nabla}^2\tilde{\omega}_A}$$

* For me: Free convection is very similar to Marangoni Flow. This may be interesting to look into more.

* Comments: Something similar happens for temperature-driven density differences:

$$Gr = \frac{g\bar{\beta}(T_1-T_0)L^3}{\nu^2}$$

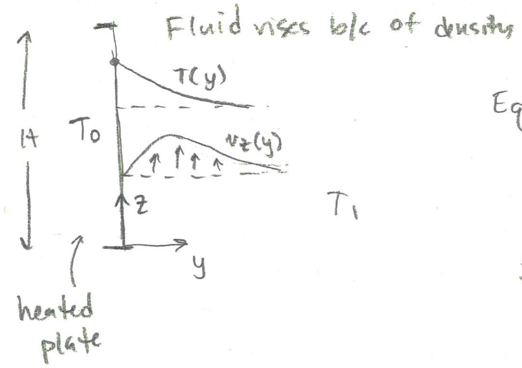
- Other dimensional bases are possible. see Table 11.5-1 (p.355, §11.5) and Eq. 19.5-8 to 19.5-11 (p.600, § 19.5)

IV. Free Convection

* with the Boussinesq approximation, we can now look at problems where density differences (due to T or ω_A gradients) can drive flow. This is called free convection. Contrast this with forced convection where pressure, boundaries, or external fields drive flow.

A. Free Convection on a vertical Flat Plate (Heat Transfer)

§11.4, Ex 11.4-5



Equations of change:

$$\nabla \cdot \underline{v} = 0$$

$$\rho \frac{D\underline{v}}{Dt} = -\nabla p + \nabla^2 \underline{v} + \rho \underline{g} \beta (T - T_1)$$

$$\rho \hat{C}_p \frac{DT}{Dt} = k \nabla^2 T$$

* Steady state, 2D: $\underline{v} = \begin{bmatrix} v_y(y,z) \\ v_z(y,z) \end{bmatrix}$, $T = T(y,z)$

$$\frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \quad , \quad v_x = 0$$

$$\rho \left(v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) = \mu \left(\frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right) + \bar{\rho} g \bar{\beta} (T - T_1) - \frac{\partial P}{\partial y}$$

$$\rho \left(v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) = \mu \left(\frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) + \bar{\rho} g \bar{\beta} (T - T_1) - \frac{\partial P}{\partial z}$$

$$\rho \hat{C}_p \left(v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)$$

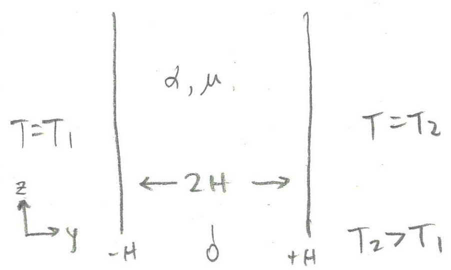
* Clearly $v_y \ll v_z$. We can justify this similar to the way we do boundary layers.

* The length scale for z is L.. For y it will be δ where $\delta \ll L$.

* Using this, these equations will reduce to the boundary layer equations! we will defer discussion of these until later in the course.

(see also Deen, ch. 12, esp. 12.4)

B. Free Convection between parallel plates (Deen 12.3-1, p. 467)



$$\frac{DT}{Dt} = \alpha \nabla^2 T$$

$$\rho \frac{D\underline{v}}{Dt} = -\underline{\nabla} \mathcal{P} + \mu \nabla^2 \underline{v} - \bar{\rho} \underline{g} \bar{\beta} (T - \bar{T})$$

* First solve for T distribution

$\nabla^2 T = 0$ at steady state

$$\frac{d^2T}{dy^2} = 0 \qquad T(-H) = T_1, \quad T(H) = T_2$$

$$T = c_1 y + c_2 \qquad T(H) = c_1 H + c_2 = T_2$$

$$T(-H) = c_1(-H) + c_2 = T_1$$

$$c_2 = \frac{T_1 + T_2}{2} \qquad c_1 = \frac{T_2 - T_1}{2H}$$

$$T = \frac{T_2 - T_1}{2H} y + \frac{T_1 + T_2}{2} \quad \checkmark$$

* Now, lets solve for the velocity distribution.

  - we will have unidirectional flow

    $v_z = v_z(y)$ only.

  - assume steady state $\Rightarrow \rho \frac{D\underline{v}}{Dt} = 0$

$$0 = -\frac{\partial P}{\partial z} + \mu \frac{\partial^2 v_z}{\partial y^2} + \rho g \beta (T - \bar{T})$$

what is $\bar{T}$?

$\frac{\partial^2 v_z}{\partial x^2} = \frac{\partial^2 v_z}{\partial z^2} = 0$ $\quad \underline{g} = [0, 0, -g]$

we haven't picked yet since there is no T_∞.

what is $\frac{\partial P}{\partial z} = ?$ If a pressure gradient exists, we will have mixed convection. lets assume $\frac{\partial P}{\partial z} = 0$. This gives us free convection only. (e.g. closed channel ends)

mixed = both free & forced convection

$$\frac{d^2 v_z}{dy^2} = -\frac{\rho g \beta}{\mu}(T - \bar{T})$$

$T = T(y)$

lets set $\bar{T} = \frac{T_1 + T_2}{2}$.

we could pick something else, but this will be convenient.

$$\frac{d^2 v_z}{dy^2} = \frac{-\rho g \beta}{\mu}\left[\frac{T_2 - T_1}{2H} y + \cancel{\frac{T_1 + T_2}{2}} - \cancel{\frac{(T_1 + T_2)}{2}}\right]$$

$$\frac{d^2 v_z}{dy^2} = -\frac{\rho g \beta \Delta T}{2 \mu H} y$$

$\Delta T = T_2 - T_1$

* integrate 2x

$$\frac{d v_z}{dy} = -\frac{\rho g \beta \Delta T}{2 \mu H}\frac{y^2}{2} + c_1 \Rightarrow v_z = -\frac{\rho g \beta \Delta T}{6 \mu H} y^3 + c_1 y + c_2$$

* Evaluate BC's:

$$v_z(-H) = 0 = -\frac{\rho g \beta \Delta T (-H)^3}{12 \mu H} + c_1(-H) + c_2$$

$$v_z(H) = 0 = -\frac{\rho g \beta \Delta T (H)^3}{12 \mu H} + c_1(H) + c_2$$

- sum : $c_2 = 0$

- diff : $\cancel{2}\cancel{H} c_1 = \frac{\cancel{2} \rho g \beta \Delta T H^{\cancel{3}}}{12 \mu \cancel{H}}$

$$c_1 = \frac{\rho g \beta H \Delta T}{12 \mu}$$

* Now, substitute back into solution

$$v_z = -\frac{\rho g \beta \Delta T}{12 \mu H} y^3 + \frac{\rho g \beta H \Delta T}{12 \mu} y$$

$$v_z = -\frac{\rho g \beta \Delta T}{12 \mu} \cdot \frac{H^{\cancel{3}\,2}}{\cancel{H}} \frac{y^3}{H^3} + \frac{\rho g \beta \Delta T}{12 \mu} H \, H \frac{y}{H}$$

$$\boxed{v_z = \frac{\rho g \beta H^2 \Delta T}{12 \mu} \left[\frac{y}{H} - \frac{y^3}{H^3} \right]}$$