Sept. 26
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Recap

Constitutive Equation relates:

Flux – Transport Property – Force Gradient

Heat: $q = -k \cdot \vec{\nabla} T$ (Fourier)

Momentum: $\tau_{yx} = \mu \frac{dv_x}{dy}$ (Newton's Law of Viscosity)

Mass: $j_A = -D_{AB} \vec{\nabla} \rho_A$ (Fick)

Unified 1D Constitutive Eq.

$$\boxed{f_y = -D \frac{db}{dy}}$$

f_y... flux of property in y direction

$\alpha = \nu = D_{AB} \equiv D$

D [=] $\frac{m^2}{s}$... diffusivity

b... property concentration

Species Diffusion

molar flux observed by stationary observer has a convective and diffusive flux component

flux relation

$$N_i = \begin{cases} C_i \vec{v} + \vec{J}_i & \text{based on mass average velocity } \vec{v} \\ C_i \vec{v}^{(M)} + \vec{J}_i^{(M)} & \text{based on molar average velocity } \vec{v}^{(M)} \end{cases}$$

Binary System, A, B

$$\boxed{N = N_A + N_B}$$ total convective flux relative to stationary observer

$$= C\,v^{(M)}\ ;\quad \boxed{C = C_A + C_B}$$ total concentration

(drop "vector" for simlicity)
i.e. consider 1D transport

$\Longrightarrow$ molar average velocity: $\boxed{v^{(M)} = \dfrac{N_A + N_B}{C}}$

We substitute $v^{(M)}$ into the flux relation: $N_i = C_i\, v^{(M)} + J_i$

$$\Longrightarrow \quad \boxed{N_A = J_A^{(M)} + \frac{C_A}{C}\left(N_A + N_B\right)}$$

Next subst. for $J_A^{(M)} = -C D_{AB} \dfrac{dx_A}{dz}$ (Fick's Law)
from Deen Table (1-3) eq. D
mole fraction

$$\Longrightarrow (1) \quad \boxed{N_A = \underbrace{- C D_{AB} \frac{dx_A}{dz}}_{\text{diffusive flux component of A}} + \underbrace{\frac{C_A}{C}\left(N_A + N_B\right)}_{\text{convective flux component}}}$$

analoguous for B:

$$(2) \quad N_B = - C D_{BA} \frac{dx_B}{dz} + \frac{C_B}{C}\left(N_A + N_B\right)$$

To solve (1) or (2) we need $N_A = f(N_B)$

Ex: $N_A = -N_B$ (equimolar counterdiff.) $\rightarrow N_A + N_B = 0$ $\Longrightarrow \boxed{N_i = J_i^{(M)}}$ $i = A, B$

(3)

Two useful reference frames in mixtures are the *mass-average velocity* $\mathbf{v}$ and the *molar-average velocity* $\mathbf{v}^{(M)}$. They are defined as

$$\mathbf{v} = \sum_{i=1}^{n} \omega_i \mathbf{v}_i, \qquad \mathbf{v}^{(M)} = \sum_{i=1}^{n} x_i \mathbf{v}_i \tag{1.2-6}$$

where ω_i and x_i are the mass fraction and mole fraction of species i, respectively, and n is the number of chemical species in the mixture. The mass and mole fractions are related to the total mass density (ρ) and total molar concentration (C) by

$$\omega_i = \frac{\rho_i}{\rho} = \frac{\rho_i}{\sum_{i=1}^{n} \rho_i}, \qquad x_i = \frac{C_i}{C} = \frac{C_i}{\sum_{i=1}^{n} C_i}. \tag{1.2-7}$$

The various diffusional fluxes defined using $\mathbf{v}$ or $\mathbf{v}^{(M)}$ are listed in Table 1-2.

Table 1-2
Flux of Species i in Various Reference Frames and Units

Reference velocity	Molar units	Mass units
$\mathbf{0}$	$\mathbf{N}_i$	$\mathbf{n}_i$
$\mathbf{v}$	$\mathbf{J}_i$	$\mathbf{j}_i$
$\mathbf{v}^{(M)}$	$\mathbf{J}_i^{(M)}$	$\mathbf{j}_i^{(M)}$

Table 1-3
Fick's Law for Binary Mixtures of A and B

Reference velocity	Mass units		Molar units	
$\mathbf{v}$	$\mathbf{j}_A = -\rho D_{AB} \nabla \omega_A$	(A)	$\mathbf{J}_A = -\frac{\rho D_{AB}}{M_A} \nabla \omega_A$	(B)
$\mathbf{v}^{(M)}$	$\mathbf{j}_A^{(M)} = -C M_A D_{AB} \nabla x_A$	(C)	$\mathbf{J}_A^{(M)} = -C D_{AB} \nabla x_A$	(D)

Heat Flux

Constitutive Eq.

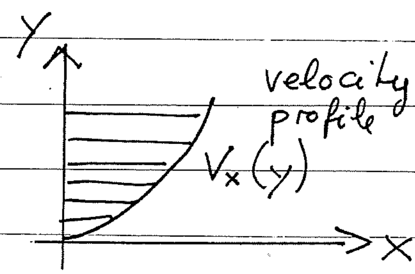
Fourier's Law: $\vec{q} = -k\,\vec{\nabla} T$; Thermal conductivity k is isotropic

$\vec{q} = -\underline{\underline{K}}\,\vec{\nabla} T$; anisotropic materials → conductivity tensor $\underline{\underline{K}}$

Heat flux normal ($\vec{n}$) to a surface :

scalar : $q_n = \vec{n} \cdot \vec{q} = -k\left(\vec{n} \cdot \vec{\nabla} T\right)$

Momentum Flux



unidirectional flow : $\vec{v} = v_x(y)\,\vec{e}_x$

⟹ Viscous stress of Newtonian fluid

$$\tau_{yx} = \mu \frac{dv_x}{dy}$$ Newton's Law of Viscosity

Newtonian fluids in 3D :

$$\underline{\underline{\tau}} = \mu\left(\underline{\underline{\nabla V}} + \left(\underline{\underline{\nabla V}}\right)^t\right)$$; t... transpose of matrix

"velocity gradient" : (velocity dyad)

$$\underline{\underline{\nabla V}} = \begin{pmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} & \frac{\partial v_x}{\partial z} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial z} & \frac{\partial v_y}{\partial z} \\ \frac{\partial v_z}{\partial x} & \frac{\partial v_z}{\partial y} & \frac{\partial v_z}{\partial z} \end{pmatrix}$$; $V_i = V_i(x, y, z)$, $i = x, y, z$