CBE 34487

6/23/20

CONTINUED DISCUSSION OF TRANSPORT EQUATIONS, APPLICATIONS AND SOLUTIONS

THE BASIC DIFFERENTIAL EQUATIONS

MOMENTUM

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}\cdot\vec{\nabla}\vec{v}\right) = -\vec{\nabla}P + \mu\nabla^2\vec{v} + \rho\vec{g}$$

x $$\rho\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = -\frac{\partial P}{\partial x} + \mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right) + \rho g_x$$

y —

z —

ENERGY

$$\rho C_p\left(\frac{\partial T}{\partial t} + V_x\frac{\partial T}{\partial x} + V_y\frac{\partial T}{\partial y} + V_z\frac{\partial T}{\partial z}\right) = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + \Phi$$

MASS:

$$\left(\frac{\partial C_A}{\partial t} + V_x\frac{\partial C_A}{\partial x} + V_y\frac{\partial C_A}{\partial y} + V_z\frac{\partial C_A}{\partial z}\right) = D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)$$

FORM OF ALL THREE EQUATIONS

RATE OF CHANGE + TRANSPORT BY CONVECTION = TRANSPORT BY DIFFUSION + SOURCES

"DIFFUSIVITY" $[=]\ \ell^2/\theta$

MOMENTUM	$\frac{\mu}{\rho} = \nu$
HEAT	$\frac{k}{\rho C_p} = \alpha$
MASS	D_{AB}

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \vec{\nabla} \vec{v} = \nu \nabla^2 \vec{v} - \frac{1}{\rho}\left[\vec{\nabla} p - \rho \vec{g}\right]$$

$$\frac{\partial T}{\partial t} + \vec{v} \cdot \vec{\nabla} T = \alpha \nabla^2 T + \frac{\mu}{\rho C_p} \bar{\Phi}$$

$$\frac{\partial C_A}{\partial t} + \vec{v} \cdot \vec{\nabla} C_A = D_{AB} \nabla^2 C_A - k C_A$$

WE CAN NON-DIMENSIONALIZE

U – CHARACTERISTIC VELOCITY

L – DIAMETER OR LENGTH

$$\frac{\partial \vec{v}^*}{\partial t^*} + \vec{v}^* \cdot \vec{\nabla}^* \vec{v}^* = \frac{\nu}{U D}\left(\nabla^{*2} \vec{v}^* - \vec{\nabla}^* p^*\right) + \frac{g L}{U^2} g^*$$

$$Re \equiv \frac{U D \rho}{\mu}, \quad Fr \equiv \frac{U^2}{g L}$$

$$\frac{\partial T^*}{\partial t^*} + \vec{v}^* \cdot \vec{\nabla}^* T^* = \frac{1}{Pe} \nabla^{*2} T^*$$

$$T^* \equiv \frac{T - T_0}{T_1 - T_0} \qquad Pe \equiv \frac{UL}{\alpha}$$

$$\frac{\partial C_A^*}{\partial t^*} = \vec{v}^* \cdot \vec{\nabla}^* C_A^* = \frac{1}{Pe_m} \nabla^{*2} C_A^* - D_A C_A^*$$

$$C_A^* = \frac{C_A}{C_{A0}} \qquad Pe_m = \frac{UL}{D_{AB}}$$

$$D_A \equiv \frac{k L^2}{D_{AB}}$$

* IMPORTANT POINT

EVENTHOUGH OUR INITIAL DERIVATIONS ARE FOR PURE SUBSTANCES, IT IS USUALLY POSSIBLE TO DEFINE "EFFECTIVE" DIFFUSIVITIES THAT DESCRIBE HETEROGENEOUS SUBSTANCES....

→ DIFFUSION OF GAS THROUGH A MEMBRANE, OR POROUS SUBSTANCE.

→ FLOW OF LIQUID THROUGH POROUS SOLID (OIL → SANDSTONE)

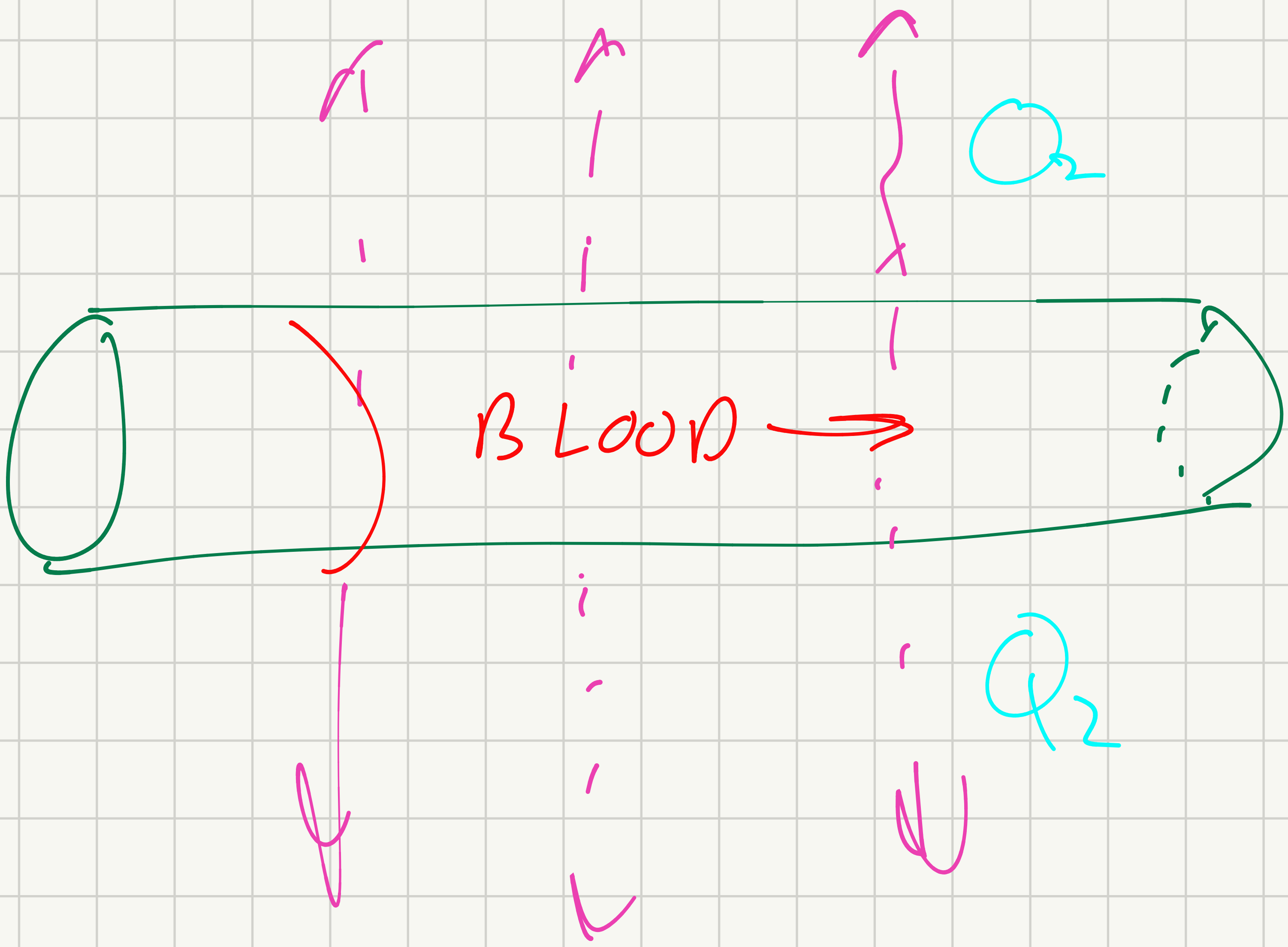
→ HEAT THROUGH INSULATION

SIZE OF A CELL

SPACING OF CAPILLARIES

DETERMINED BY RATE

OF DIFFUSION



MASS DIFFUSIVITIES
TYPICAL VALUES

SMALL MOLECULE IN ~WATER

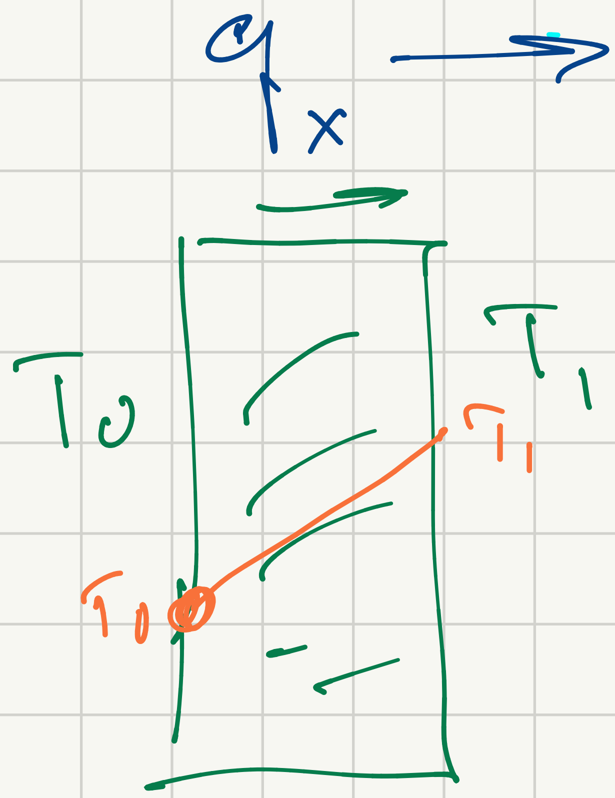
$$D \sim 10^{-5}\ cm^2/s$$

DIFFUSION OF GASES

$$D \sim 10^{-1}\ cm^2/s$$

WE ARE INTERESTED IN STEADY-STATE & TRANSIENT SITUATIONS

STEADY STATE



$$\cancel{\frac{\partial T^*}{\partial t^*}}^{0} + \cancel{\vec{V}^* \cdot \vec{\nabla}^* T^*}^{0} = \frac{1}{Pe} \nabla^{*2} T^*$$

$$\frac{\partial^2 T}{\partial x^2}, \quad T(0) = T_0, \quad T(L) = T_1$$

$$\frac{d}{dx}\frac{dT}{dx} = 0$$

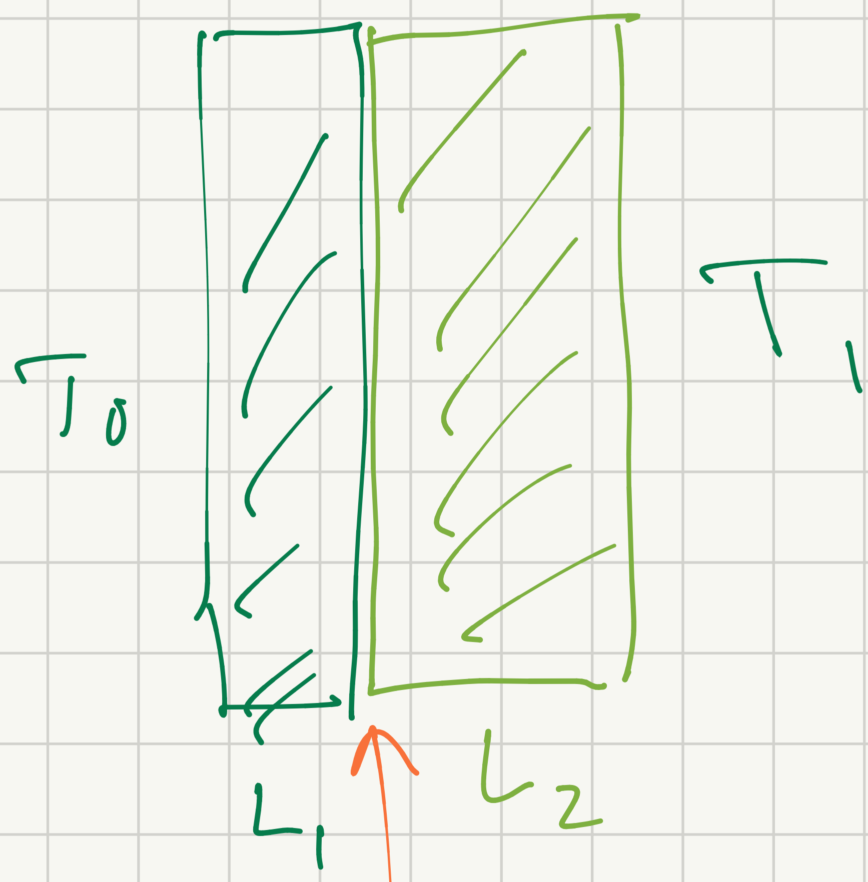
$$\frac{dT}{dx} = C_1$$

$$T = C_1 x + C_2$$

$$= \qquad T = T_0 + \frac{T_1 - T_0}{L} x$$

LINEAR PROFILE

α DOES NOT APPEAR



FLUX IN EACH MATERIAL MUST MATCH

$$k_\alpha \frac{\partial T}{\partial x} = k_\beta \frac{\partial T}{\partial x}$$

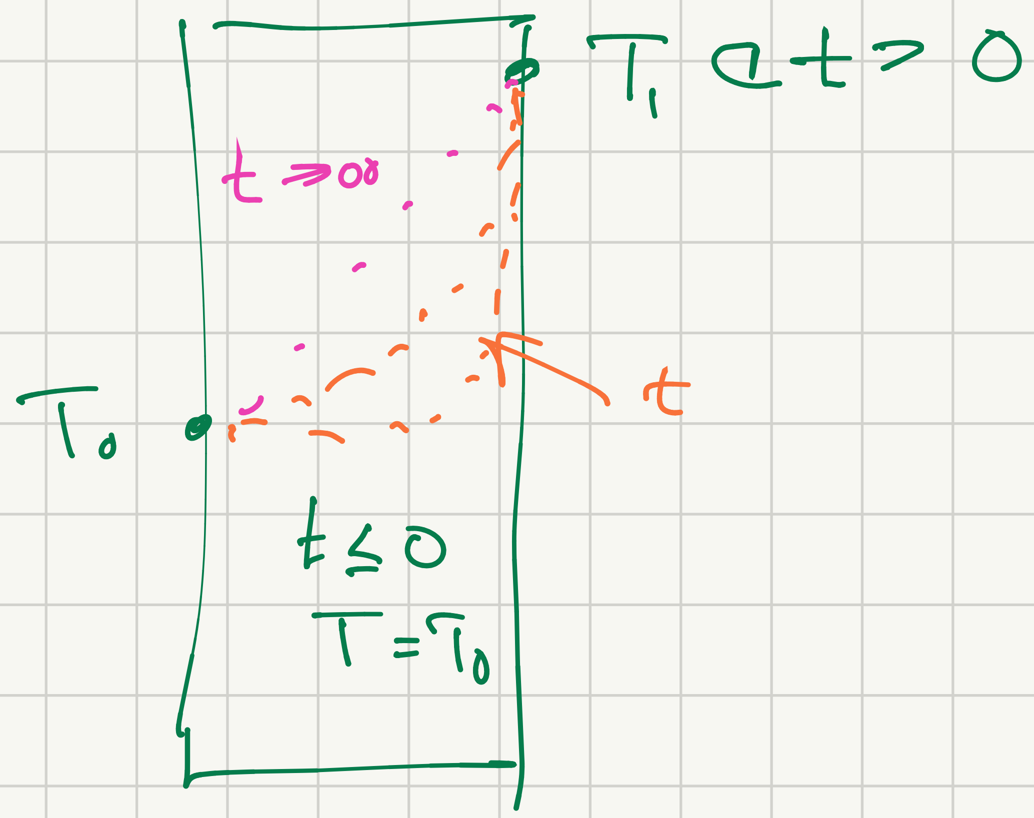
$$k_\alpha \frac{T_0 - T_i}{L_1} = k_\beta \frac{(T_i - T_1)}{L_2}$$

$$T_i = \frac{k_\alpha L_2 T_0 + k_\beta L_1 T_1}{k_\beta L_1 + k_\alpha L_2}$$

$T =$ SEE MMA.

EVEN A "SIMPLE" PROBLEM . . .
DON'T DO ALGEBRA!!

TRANSIENT DIFFUSION OR CONDUCTION



"HEAT" EQUATION

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

I.C. $T = T_0$ $t \le 0$
B.C. $T = T_0$ @ $x = 0$
$T = T_1$ @ $x = L$

"PARABOLIC" PDE.

SOLVE A PDE BY TURNING IT INTO AN ODE

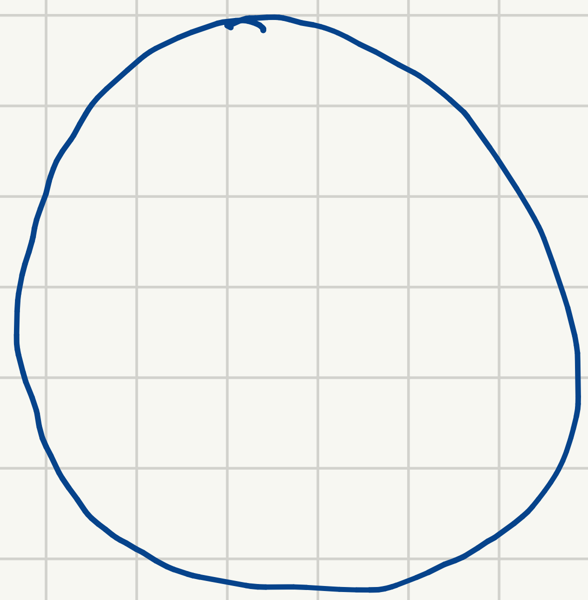
NEED TO BE ABLE TO MATCH ANY INITIAL PROFILE

→ SET OF ORTHOGONAL FUNCTIONS THAT MATCH BOUNDARY CONDITIONS

"EIGEN FUNCTIONS" + EIGEN VALUES

(SAME IDEA FOR SPECTRAL NUMERICAL METHODS)

$C_A = C_A^{\infty}$



CATALYST

$$\frac{\partial C_A}{\partial t} = D_{AB} \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial C_A}{\partial r}\right) - k C_A$$

$$Da = \frac{k R^2}{D_{AB}}$$

DIFFUSION OF CO_2 INTO A SPHERICAL PARTICLE

$$CO_2 + \text{IONIC LIQUID} \rightleftharpoons CO_2\text{—}NH_3\text{—}IL$$

USED FOR SCRUBBING CO_2 IN A FLUIDIZED BED.