

QUICK START

- Just like { momentum use
energy

"slash + burn"

- need to use micro-balance,
+ transport law
- solve for distribution of
transporting property in space, time

(TOTAL) MASS / MOMENTUM

0.2

The Equation of Continuity and the Equation of Motion in Cartesian, cylindrical, and spherical coordinates

CM3110 Fall 2011 Faith A. Morrison

Continuity Equation, Cartesian coordinates

$$\frac{\partial \rho}{\partial t} + \left(v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} \right) + \rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) = 0$$

Continuity Equation, cylindrical coordinates

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial(\rho r v_r)}{\partial r} + \frac{1}{r} \frac{\partial(\rho v_\theta)}{\partial \theta} + \frac{\partial(\rho v_z)}{\partial z} = 0$$

Continuity Equation, spherical coordinates

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial(\rho r^2 v_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\rho v_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial(\rho v_\phi)}{\partial \phi} = 0$$

Equation of Motion for an incompressible fluid, 3 components in Cartesian coordinates

$$\begin{aligned} \rho \left(\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right) &= -\frac{\partial P}{\partial x} + \left(\frac{\partial \tilde{\tau}_{xx}}{\partial x} + \frac{\partial \tilde{\tau}_{yx}}{\partial y} + \frac{\partial \tilde{\tau}_{zx}}{\partial z} \right) + \rho g_x \\ \rho \left(\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) &= -\frac{\partial P}{\partial y} + \left(\frac{\partial \tilde{\tau}_{xy}}{\partial x} + \frac{\partial \tilde{\tau}_{yy}}{\partial y} + \frac{\partial \tilde{\tau}_{zy}}{\partial z} \right) + \rho g_y \\ \rho \left(\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) &= -\frac{\partial P}{\partial z} + \left(\frac{\partial \tilde{\tau}_{xz}}{\partial x} + \frac{\partial \tilde{\tau}_{yz}}{\partial y} + \frac{\partial \tilde{\tau}_{zz}}{\partial z} \right) + \rho g_z \end{aligned}$$

Equation of Motion for an incompressible fluid, 3 components in cylindrical coordinates

$$\begin{aligned} \rho \left(\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_z \frac{\partial v_r}{\partial z} \right) &= -\frac{\partial P}{\partial r} + \left(\frac{1}{r} \frac{\partial(r \tilde{\tau}_{rr})}{\partial r} + \frac{1}{r} \frac{\partial \tilde{\tau}_{\theta r}}{\partial \theta} - \frac{\tilde{\tau}_{\theta\theta}}{r} + \frac{\partial \tilde{\tau}_{zr}}{\partial z} \right) + \rho g_r \\ \rho \left(\frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\theta v_r}{r} + v_z \frac{\partial v_\theta}{\partial z} \right) &= -\frac{1}{r} \frac{\partial P}{\partial \theta} + \left(\frac{1}{r^2} \frac{\partial(r^2 \tilde{\tau}_{r\theta})}{\partial r} + \frac{1}{r} \frac{\partial \tilde{\tau}_{\theta\theta}}{\partial \theta} + \frac{\partial \tilde{\tau}_{z\theta}}{\partial z} + \frac{\tilde{\tau}_{\theta r} - \tilde{\tau}_{r\theta}}{r} \right) + \rho g_\theta \\ \rho \left(\frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right) &= -\frac{\partial P}{\partial z} + \left(\frac{1}{r} \frac{\partial(r \tilde{\tau}_{rz})}{\partial r} + \frac{1}{r} \frac{\partial \tilde{\tau}_{\theta z}}{\partial \theta} + \frac{\partial \tilde{\tau}_{zz}}{\partial z} \right) + \rho g_z \end{aligned}$$

Equation of Motion for an incompressible fluid, 3 components in spherical coordinates

$$\begin{aligned} &\rho \left(\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_r}{\partial \phi} - \frac{v_\theta^2 + v_\phi^2}{r} \right) \\ &= -\frac{\partial P}{\partial r} + \left(\frac{1}{r^2} \frac{\partial(r^2 \tilde{\tau}_{rr})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\tilde{\tau}_{\theta r} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \tilde{\tau}_{\phi r}}{\partial \phi} - \frac{\tilde{\tau}_{\theta\theta} + \tilde{\tau}_{\phi\phi}}{r} \right) + \rho g_r \\ &\rho \left(\frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} + \frac{v_r v_\theta}{r} - \frac{v_\phi^2 \cot \theta}{r} \right) \\ &= -\frac{1}{r} \frac{\partial P}{\partial \theta} + \left(\frac{1}{r^3} \frac{\partial(r^3 \tilde{\tau}_{r\theta})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\tilde{\tau}_{\theta\theta} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \tilde{\tau}_{\phi\theta}}{\partial \phi} + \frac{\tilde{\tau}_{\theta r} - \tilde{\tau}_{r\theta}}{r} - \frac{\tilde{\tau}_{\phi\phi} \cot \theta}{r} \right) + \rho g_\theta \\ &\rho \left(\frac{\partial v_\phi}{\partial t} + v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_r v_\phi}{r} + \frac{v_\theta v_\phi \cot \theta}{r} \right) \\ &= -\frac{1}{r \sin \theta} \frac{\partial P}{\partial \phi} + \left(\frac{1}{r^3} \frac{\partial(r^3 \tilde{\tau}_{r\phi})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\tilde{\tau}_{\theta\phi} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \tilde{\tau}_{\phi\phi}}{\partial \phi} + \frac{\tilde{\tau}_{\phi r} - \tilde{\tau}_{r\phi}}{r} + \frac{\tilde{\tau}_{\phi\theta} \cot \theta}{r} \right) + \rho g_\phi \end{aligned}$$

The Newtonian Constitutive Equation in Cartesian, Cylindrical, and Spherical coordinates

Prof. Faith A. Morrison, Michigan Technological University

Cartesian Coordinates

$$\begin{pmatrix} \tilde{\tau}_{xx} & \tilde{\tau}_{xy} & \tilde{\tau}_{xz} \\ \tilde{\tau}_{yx} & \tilde{\tau}_{yy} & \tilde{\tau}_{yz} \\ \tilde{\tau}_{zx} & \tau_{zy} & \tilde{\tau}_{zz} \end{pmatrix}_{xyz} = \mu \begin{pmatrix} 2 \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} & \frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \\ \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} & 2 \frac{\partial v_y}{\partial y} & \frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \\ \frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} & \frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} & 2 \frac{\partial v_z}{\partial z} \end{pmatrix}_{xyz}$$

Cylindrical Coordinates

$$\begin{pmatrix} \tilde{\tau}_{rr} & \tilde{\tau}_{r\theta} & \tilde{\tau}_{rz} \\ \tilde{\tau}_{\theta r} & \tilde{\tau}_{\theta\theta} & \tilde{\tau}_{\theta z} \\ \tilde{\tau}_{zr} & \tau_{z\theta} & \tilde{\tau}_{zz} \end{pmatrix}_{r\theta z} = \mu \begin{pmatrix} 2 \frac{\partial v_r}{\partial r} & r \frac{\partial}{\partial r} \left(\frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} & \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \\ r \frac{\partial}{\partial r} \left(\frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} & 2 \left(\frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) & \frac{1}{r} \frac{\partial v_z}{\partial \theta} + \frac{\partial v_\theta}{\partial z} \\ \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} & \frac{1}{r} \frac{\partial v_z}{\partial \theta} + \frac{\partial v_\theta}{\partial z} & 2 \frac{\partial v_z}{\partial z} \end{pmatrix}_{r\theta z}$$

Spherical Coordinates

$$\begin{pmatrix} \tilde{\tau}_{rr} & \tilde{\tau}_{r\theta} & \tilde{\tau}_{r\phi} \\ \tilde{\tau}_{\theta r} & \tilde{\tau}_{\theta\theta} & \tilde{\tau}_{\theta\phi} \\ \tilde{\tau}_{\phi r} & \tau_{\phi\theta} & \tilde{\tau}_{\phi\phi} \end{pmatrix}_{r\theta\phi} = \mu \begin{pmatrix} 2 \frac{\partial v_r}{\partial r} & r \frac{\partial}{\partial r} \left(\frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} & \frac{1}{r \sin \theta} \frac{\partial v_r}{\partial \phi} + r \frac{\partial}{\partial r} \left(\frac{v_\phi}{r} \right) \\ r \frac{\partial}{\partial r} \left(\frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} & 2 \left(\frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) & \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(\frac{v_\phi}{\sin \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} \\ \frac{1}{r \sin \theta} \frac{\partial v_r}{\partial \phi} + r \frac{\partial}{\partial r} \left(\frac{v_\phi}{r} \right) & \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(\frac{v_\phi}{\sin \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} & 2 \left(\frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_r}{r} + \frac{v_\theta \cot \theta}{r} \right) \end{pmatrix}_{r\theta\phi}$$

These expressions are general and are applicable to three-dimensional flows. For unidirectional flows they reduce to Newton's law of Viscosity. Reference: Faith A. Morrison, *An Introduction to Fluid Mechanics* (Cambridge University Press: New York, 2013)

— ENERGY —

0.4

The **Equation of Energy** in Cartesian, cylindrical, and spherical coordinates for Newtonian fluids of constant density, with source term S_e . Source could be electrical energy due to current flow, chemical energy, etc. Two cases are presented: the general case where thermal conductivity may be a function of temperature (vector flux $\tilde{q} = q/\text{area}$ appears in the equations); and the more usual case, where thermal conductivity is constant (on the reverse).

Spring 2020 Faith A. Morrison, Michigan Technological University

Microscopic energy balance, in terms of flux; Gibbs notation

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = -\nabla \cdot \tilde{q} + S_e$$

Microscopic energy balance, in terms of flux; Cartesian coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = - \left(\frac{\partial \tilde{q}_x}{\partial x} + \frac{\partial \tilde{q}_y}{\partial y} + \frac{\partial \tilde{q}_z}{\partial z} \right) + S_e$$

Microscopic energy balance, in terms of flux; cylindrical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = - \left(\frac{1}{r} \frac{\partial (r \tilde{q}_r)}{\partial r} + \frac{1}{r} \frac{\partial \tilde{q}_\theta}{\partial \theta} + \frac{\partial \tilde{q}_z}{\partial z} \right) + S_e$$

Microscopic energy balance, in terms of flux; spherical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial T}{\partial \phi} \right) = - \left(\frac{1}{r^2} \frac{\partial (r^2 \tilde{q}_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial (\tilde{q}_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \tilde{q}_\phi}{\partial \phi} \right) + S_e$$

Fourier's law of heat conduction, Gibbs notation: $\tilde{q} = q/A = -k \nabla T$

Fourier's law of heat conduction, Cartesian coordinates:
(constant thermal conductivity k)

$$\begin{pmatrix} \tilde{q}_x \\ \tilde{q}_y \\ \tilde{q}_z \end{pmatrix}_{xyz} = \begin{pmatrix} q_x/A \\ q_y/A \\ q_z/A \end{pmatrix}_{xyz} = \begin{pmatrix} -k \frac{\partial T}{\partial x} \\ -k \frac{\partial T}{\partial y} \\ -k \frac{\partial T}{\partial z} \end{pmatrix}_{xyz}$$

Fourier's law of heat conduction, cylindrical coordinates:
(constant thermal conductivity k)

$$\begin{pmatrix} \tilde{q}_r \\ \tilde{q}_\theta \\ \tilde{q}_z \end{pmatrix}_{r\theta z} = \begin{pmatrix} q_r/A \\ q_\theta/A \\ q_z/A \end{pmatrix}_{r\theta z} = \begin{pmatrix} -k \frac{\partial T}{\partial r} \\ -\frac{k}{r} \frac{\partial T}{\partial \theta} \\ -k \frac{\partial T}{\partial z} \end{pmatrix}_{r\theta z}$$

Fourier's law of heat conduction, spherical coordinates:
(constant thermal conductivity k)

$$\begin{pmatrix} \tilde{q}_r \\ \tilde{q}_\theta \\ \tilde{q}_\phi \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} q_r/A \\ q_\theta/A \\ q_\phi/A \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} -k \frac{\partial T}{\partial r} \\ -\frac{k}{r} \frac{\partial T}{\partial \theta} \\ -\frac{k}{r \sin \theta} \frac{\partial T}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

Energy Transport Law

SPECIES A MASS (in a mixture)

0.5

The Equation of Species Mass Balance in Terms of Combined Molar quantities

in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the combined molar flux with respect to molar velocity (\underline{N}_A), is given on page 1.

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In terms of total molar flux, \underline{N}_A

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

WRF 25-11

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r} \frac{\partial(rN_{A,r})}{\partial r} + \frac{1}{r} \frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2} \frac{\partial(r^2 N_{A,r})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(N_{A,\theta} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

WRF 24-22

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

Fick's law of diffusion, Cartesian coordinates: $\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB} \frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB} \frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$

Fick's law of diffusion, cylindrical coordinates: $\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$

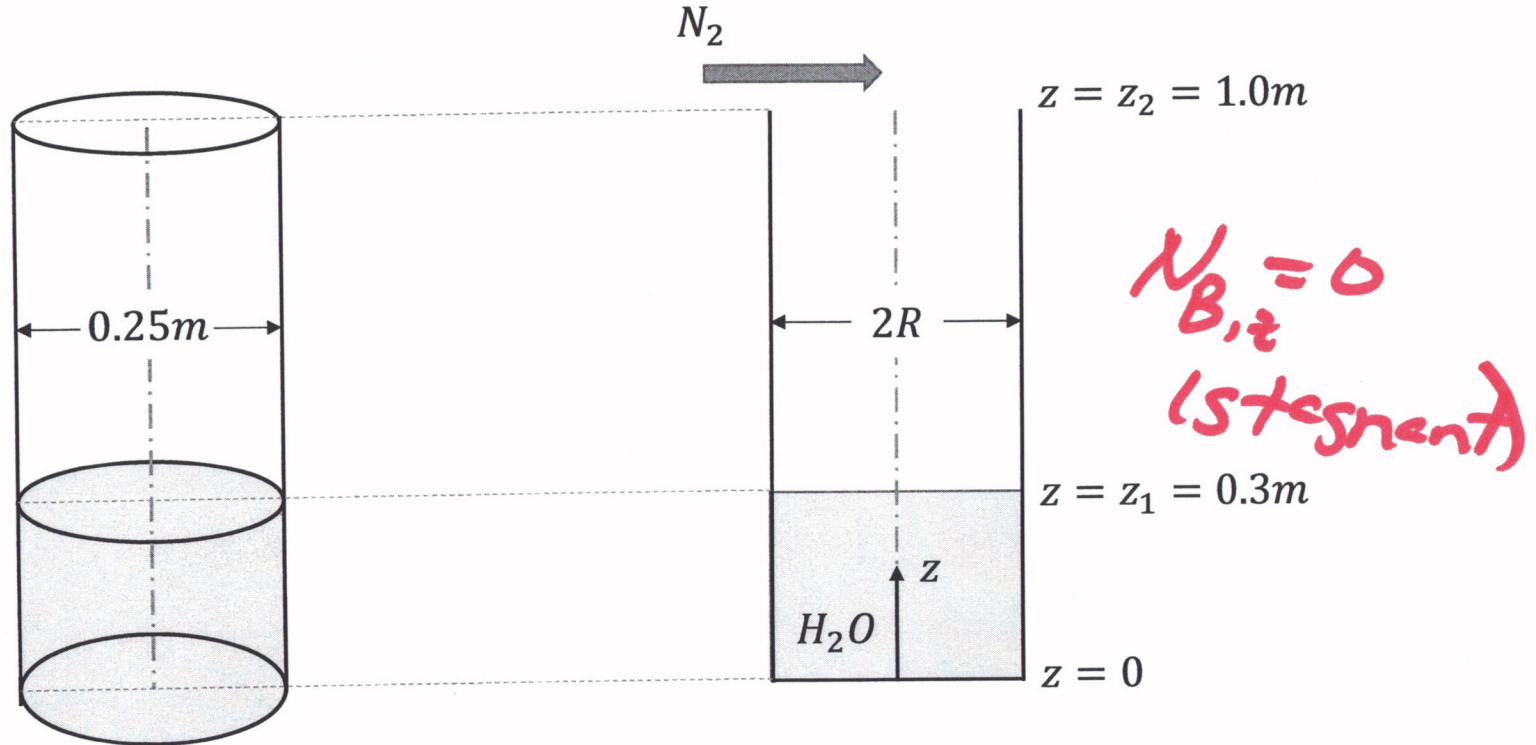
Fick's law of diffusion, spherical coordinates: $\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$

SPECIES A TRANSPORT LAW

1D Evaporation from tank

QUICK START

Example 1: Water (40°C , 1.0 atm) slowly and steadily evaporates into nitrogen (40°C , 1.0 atm) from the bottom of a cylindrical tank as shown in the figure below. A stream of dry nitrogen flows slowly past the open tank. The mole fraction of water in the gas at the top opening of the tank is 0.02. The geometry is as shown in the figure. **What is the rate of water evaporation?**



The Equation of Species Mass Balance in Terms of Combined Molar quantities

in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B. The general case, where the combined molar flux with respect to molar velocity (\underline{N}_A), is given on page 1.

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In terms of total molar flux, \underline{N}_A

Microscopic species mass balance, in terms of molar flux; Gibbs notation

Assume this (start simple)

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

WRF 25-11

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

1D mass flux

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r} \frac{\partial(r N_{A,r})}{\partial r} + \frac{1}{r} \frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

no reaction

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

steady

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2} \frac{\partial(r^2 N_{A,r})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(N_{A,\theta} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

symmetry

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

WRF 24-22

Handwritten box:

$$\frac{\partial N_{A,z}}{\partial z} = 0$$

$$x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} = 0$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB} \frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB} \frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}$$

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

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In terms of total molar flux, \underline{N}_A

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

WRF 25-11

Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r} \frac{\partial(rN_{A,r})}{\partial r} + \frac{1}{r} \frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2} \frac{\partial(r^2 N_{A,r})}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(N_{A,\theta} \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

WRF 24-22

$$= c_A \underline{v}^* - cD_{AB}\nabla x_A$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB} \frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB} \frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

all undastood

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB} \frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB} \frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r} \frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r \sin \theta} \frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

Statement

1 NO sink => NO flux

④

$$\frac{dN_{A,z}}{dz} = 0$$

⇒ constant flux

$$N_{A,z} = C_1$$

flux:

$$N_{A,z} = \frac{\text{mols A}}{\text{time} \cdot \text{area}} = \text{constant}$$

Fick's Law (stagnant B)

$$N_{A,z} = x_A N_{A,z} - c D_{AB} \frac{dx_A}{dz}$$

Solve for $x_A(z)$:

$$N_{A,z}(1 - x_A) = -c D_{AB} \frac{dx_A}{dz}$$

$$\int \underbrace{\left(\frac{-N_{A2}}{CD_{AB}} \right)}_{\text{constants}} dz = (-1) \int \frac{-dx_A}{(1-x_A)}$$

$$\left(\frac{-N_{A2}}{CD_{AB}} \right) z = \int$$

$$u = 1 - x_A$$

$$du = -dx_A$$

$$= -\ln(1-x_A) + C_2$$

C₂
second
integration
constant

BC: (What are
the boundaries?)
solve.

(Will finish
next time)

G