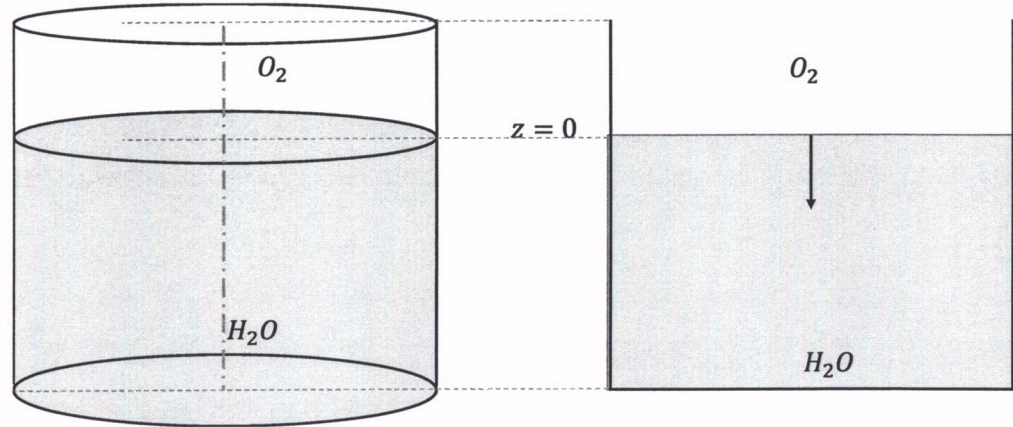


Example 14: A very long, very wide tank of water is suddenly exposed to oxygen atmosphere. Oxygen diffuses into the water. What is the concentration profile of the oxygen in the water as a function of time?

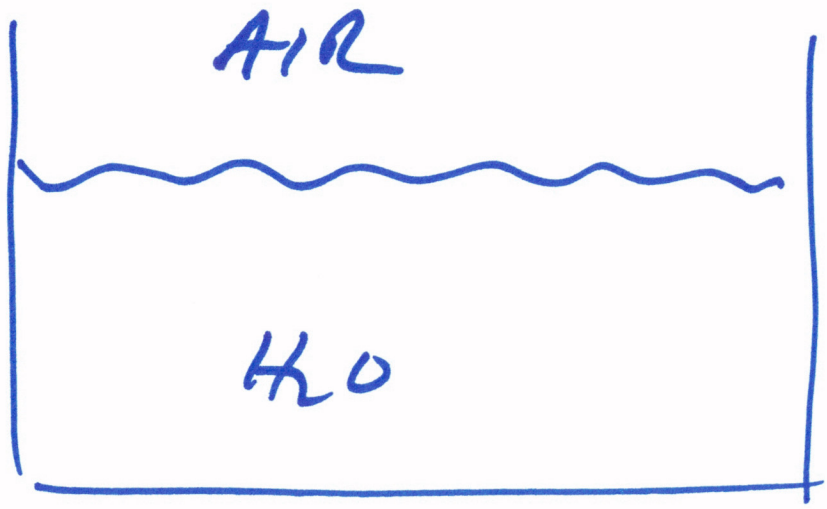


A ⇒ MICRO SPECIES MASS BAL

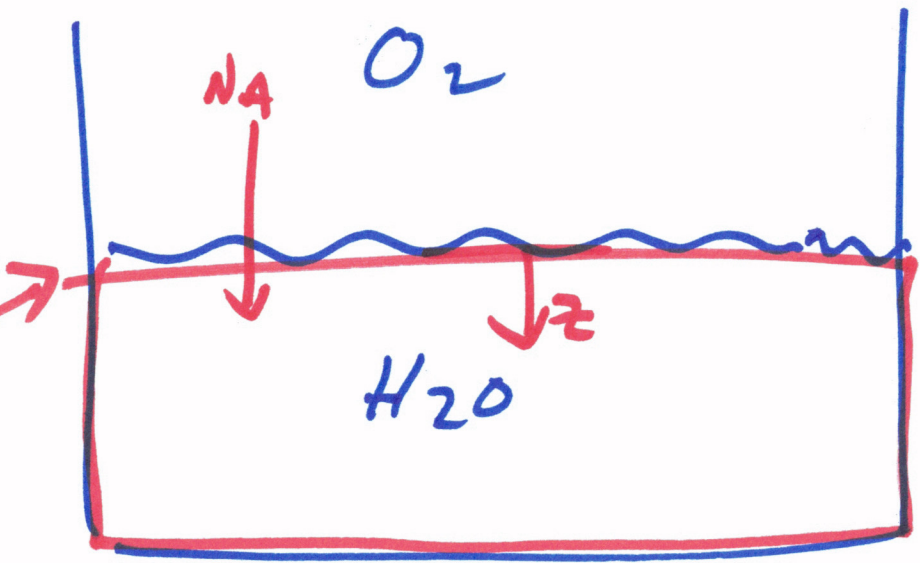
You try.

assume:
low mass
xfr rates

Initially



Suddenly



Cartesian $x_A(z)$

domain:

water

$-\infty < z < \infty$

$z=0$

$w_A = w_A^*$

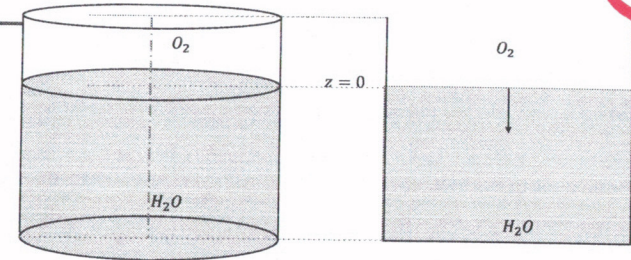
$z=\infty$

$w_A = 0$
 w_m

What is conc. dist O₂ in water as a function of time?

⇒ microscopic

2.5



Which microscopic species
A mass balance is best for
solving the model?

Various forms of Fick's Law (and the species mass balances that employ them)

Mass flux	Molar flux	Combined molar flux
$\underline{j}_A = -\rho D_{AB} \nabla \omega_A$	$\underline{J}_A^* = -c D_{AB} \nabla x_A$	$\underline{N}_A = x_A (\underline{N}_A + \underline{N}_B) - c D_{AB} \nabla x_A$

FRONT

need to separate bulk + diffusive motions



The **Equation of Species Mass Balance, constant ρD_{AB}** . For binary systems, and Fick's law has been incorporated. Good for dilute liquid solutions at constant temperature and pressure.

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$\rho \left(\frac{\partial \omega_A}{\partial t} + \underline{v} \cdot \nabla \omega_A \right) = \rho D_{AB} \nabla^2 \omega_A + r_A$$

chose mass units

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$\rho \left(\frac{\partial \omega_A}{\partial t} + v_x \frac{\partial \omega_A}{\partial x} + v_y \frac{\partial \omega_A}{\partial y} + v_z \frac{\partial \omega_A}{\partial z} \right) = \rho D_{AB} \left(\frac{\partial^2 \omega_A}{\partial x^2} + \frac{\partial^2 \omega_A}{\partial y^2} + \frac{\partial^2 \omega_A}{\partial z^2} \right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$\rho \left(\frac{\partial \omega_A}{\partial t} + v_r \frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r} \frac{\partial \omega_A}{\partial \theta} + v_z \frac{\partial \omega_A}{\partial z} \right) = \rho D_{AB} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \omega_A}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \omega_A}{\partial \theta^2} + \frac{\partial^2 \omega_A}{\partial z^2} \right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$\rho \left(\frac{\partial \omega_A}{\partial t} + v_r \frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r} \frac{\partial \omega_A}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial \omega_A}{\partial \phi} \right) = \rho D_{AB} \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \omega_A}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \omega_A}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \omega_A}{\partial \phi^2} \right) + r_A$$

In terms of Diffusivity, D_{AB}

$$c x_A = c_A = \frac{1}{M_A} (\rho_A) = \frac{1}{M_A} (\rho \omega_A) \quad \left(\text{units: } c [=] \frac{\text{mol mix}}{\text{vol soln}}; \rho [=] \frac{\text{mass mix}}{\text{vol soln}}; c_A [=] \frac{\text{mol A}}{\text{vol soln}}; \rho_A [=] \frac{\text{mass A}}{\text{vol soln}} \right)$$

$$\underline{J}_A \equiv \text{mass flux of species } A \text{ relative to a mixture's mass average velocity, } \underline{v} \quad \left(\text{units: } \underline{J}_A [=] \frac{\text{mass } A}{\text{area} \cdot \text{time}} \right)$$

$$= \rho_A (\underline{v}_A - \underline{v})$$

$\underline{J}_A + \underline{J}_B = 0$, i.e. these fluxes are measured relative to the mixture's center of mass

$\underline{n}_A \equiv \rho_A \underline{v}_A = \underline{J}_A + \rho_A \underline{v} =$ combined mass flux relative to stationary coordinates

$$\underline{n}_A + \underline{n}_B = \rho \underline{v}$$

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v} = \omega_A \underline{v}_A + \omega_B \underline{v}_B \equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002. (p. 515, 584)

Diffusion
eqn:

$$\frac{\partial W_A}{\partial t} = D_{AB} \frac{\partial^2 W_A}{\partial z^2}$$

$$0 < z < \infty \quad \textcircled{1}$$

Initial condition: $t < 0$

$$W_A = 0 \quad \forall z$$

W_{A0} "bulk"

Boundary conditions:

$$z = 0 \quad W_A = W_A^* \quad \forall t > 0$$

$$z = \infty \quad W_A = 0$$

W_{A0}

Note: $C_A = \underbrace{\frac{\rho}{M_A}}_{\text{constant}} W_A$

$$\Rightarrow \frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial z^2}$$

(true for $\textcircled{1}$ ideal
gases & $\textcircled{2}$
dilute solns since C must be constant)

We've seen this
mathematics before!