ChE-402: Diffusion and Mass Transfer

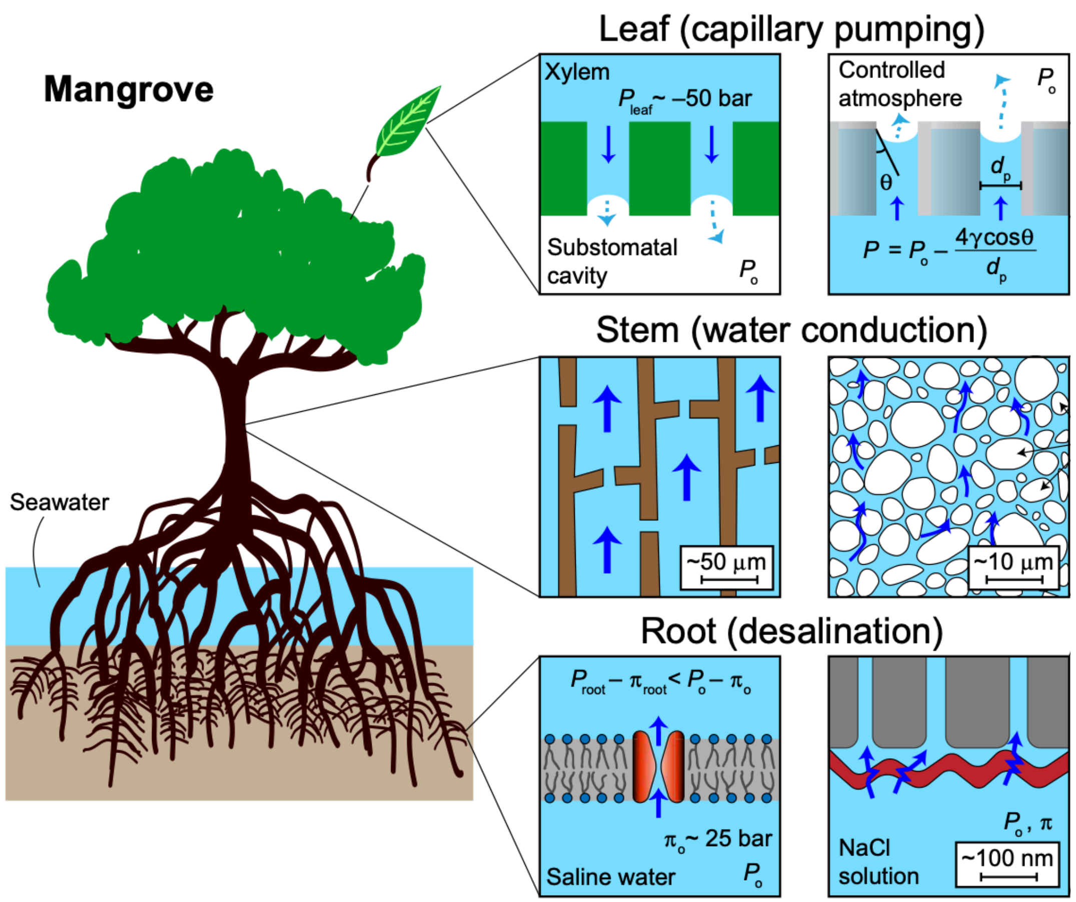
Lecture 4

Intended Learning Outcome

- To solve steady-state problems involving both convection and diffusion.
- To further analyze the link between velocity, diffusion, and convection.

EPFL

Capillary evaporation

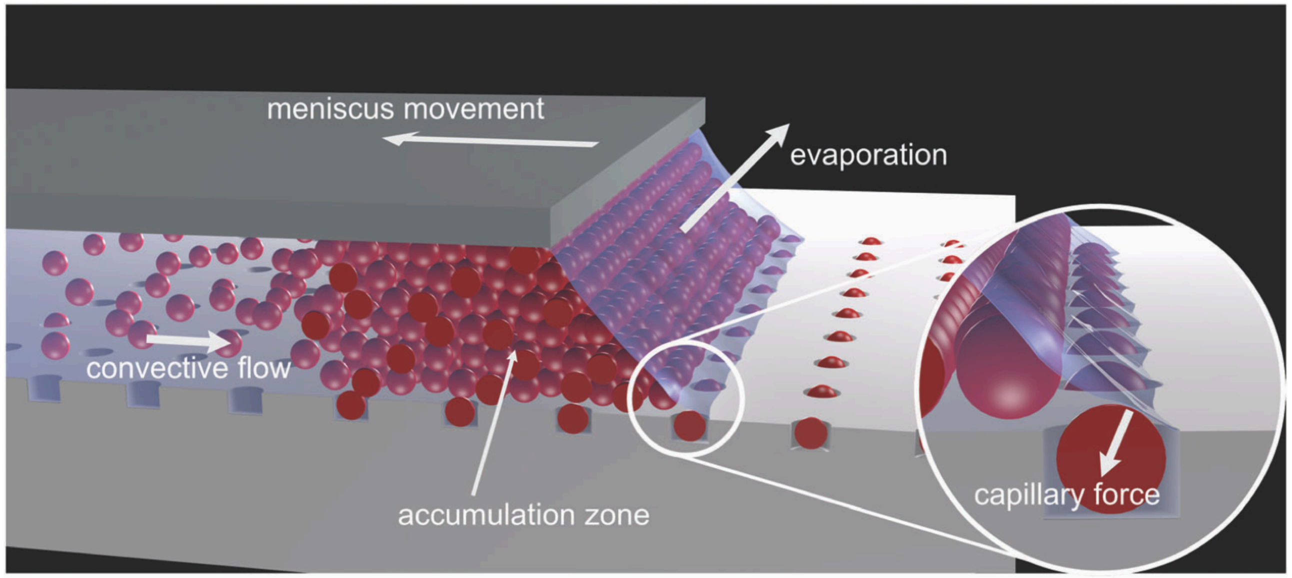


SCIENCE ADVANCES | RESEARCH ARTICLE

ENGINEERING

Capillary-driven desalination in a synthetic mangrove

Yunkun Wang[1,2], Jongho Lee[2,3], Jay R. Werber[2,4], Menachem Elimelech[2]*



Soft Matter

REVIEW

View Article Online
View Journal | View Issue

Capillary assembly as a tool for the heterogeneous integration of micro- and nanoscale objects

Songbo Ni,[ab] Lucio Isa*[b] and Heiko Wolf*[a]

Solving the evaporation problem in <u>stagnant air</u>

Calculate flux and concentration profile of evaporating benzene in stagnant air.

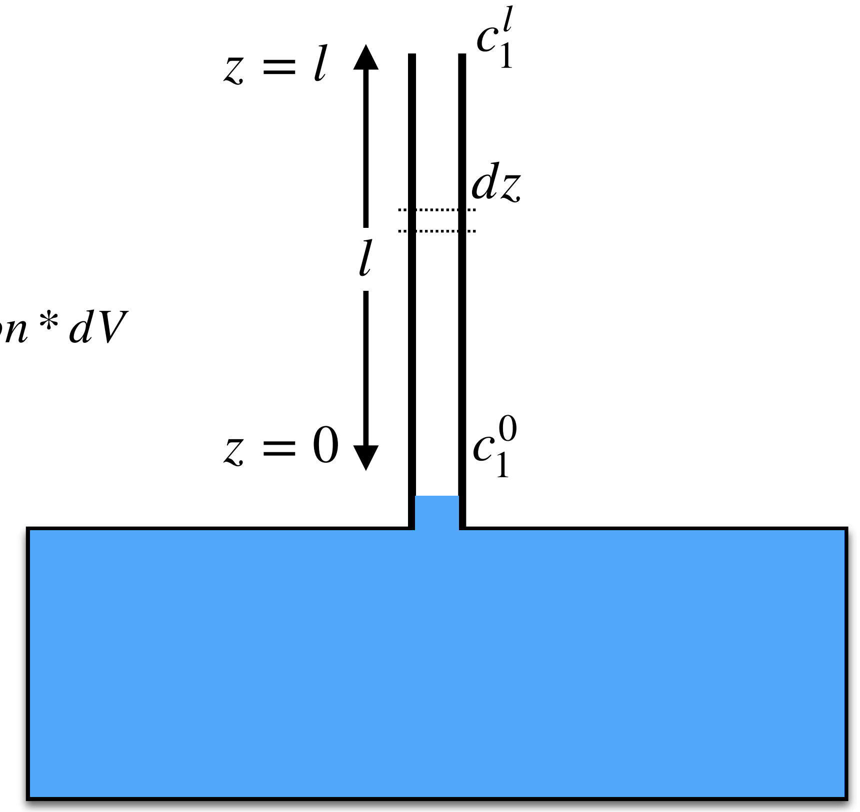
By stagnant air, we are approximating the velocity of air to be zero (total flux of air $n_2 = c_2 v_2 = 0$).

Define your system - capillary tube

Define an element to do mass balance

Apply mass balance

$$\overset{o}{Accumulation} * dV = \overset{o}{Flux}\,|_{in} * A - \overset{o}{Flux}\,|_{out} * A + \overset{o}{Generation} * dV - \overset{o}{Consumption} * dV$$



Liquid evaporation through a capillary

Solving the evaporation problem in stagnant air

Using average velocity of volumes for convective flux

$n_1 = j_1^a + c_1 v^a$ where $v^a = v^v$

$$n_1 = -D\frac{dc_1}{dz} + c_1 v^v$$

$$v^v = c_1\bar{V}_1 v_1 + c_2\bar{V}_2 v_2$$

Air is stagnant

$$\Rightarrow \quad v_2 = 0$$

$$\Rightarrow \quad v^v = c_1\bar{V}_1 v_1 = \bar{V}_1 n_1 \text{ (constant)}$$

$$n_1 = -D\frac{dc_1}{dz} + c_1(\bar{V}_1 n_1)$$

$$D\frac{dc_1}{dz} - c_1(\bar{V}_1 n_1) + n_1 = 0$$

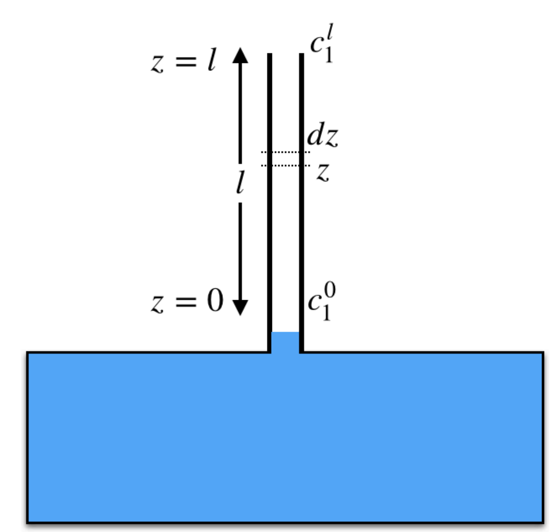
n_1 is constant

$$\frac{dc_1}{dz} - \frac{\bar{V}_1 n_1}{D}c_1 + \frac{n_1}{D} = 0$$

$\bar{V}_1 = \bar{V}_2 = \dfrac{1}{\bar{c}}$ **is constant (22.4 liter/mole) in vapor phase at 1 bar.**

Boundary conditions **(two boundary conditions for ODE because n_1 is also unknown)**

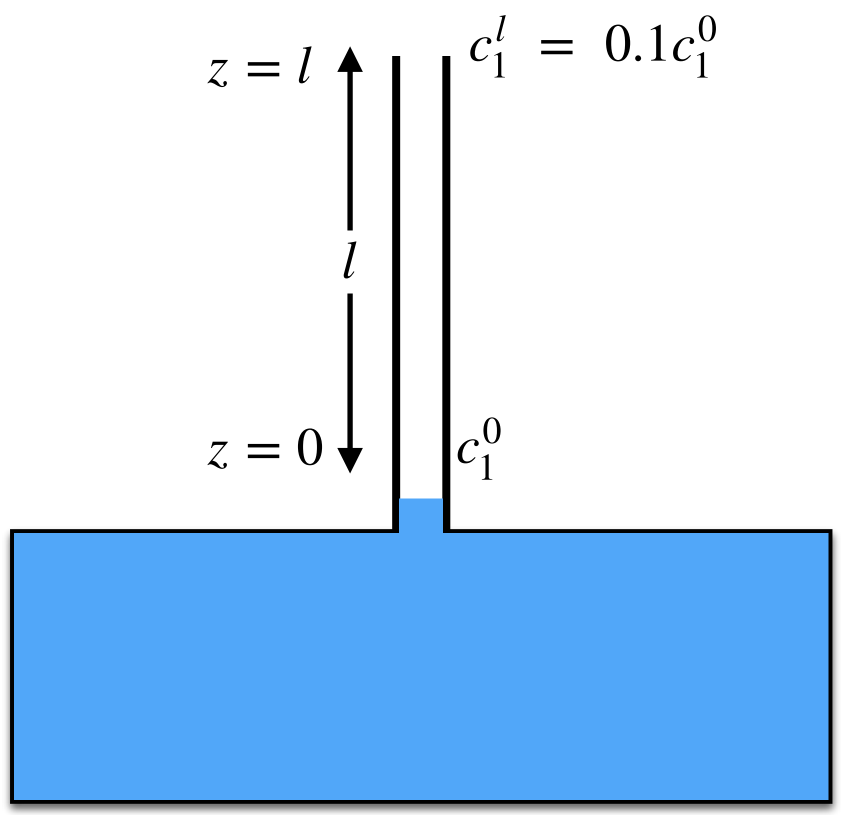
$$\boxed{\frac{\bar{c} - c_1}{\bar{c} - c_1^0} = \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} \qquad n_1 = \frac{D\bar{c}}{l}\ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)}$$



Liquid evaporation through a capillary

Where is the velocity maximum in this case

A. Top (z = L)
B. Bottom (z = 0)
C. Not enough information
D. Velocity is constant



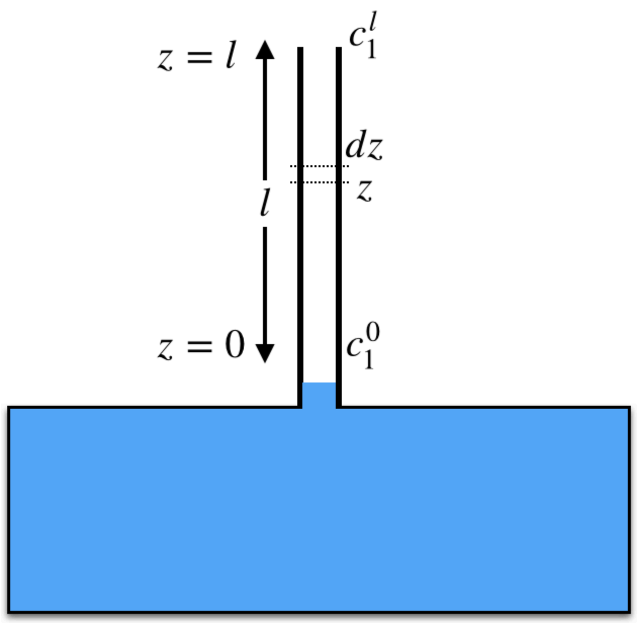
Liquid evaporation through a capillary

Relative contribution of diffusion and convection

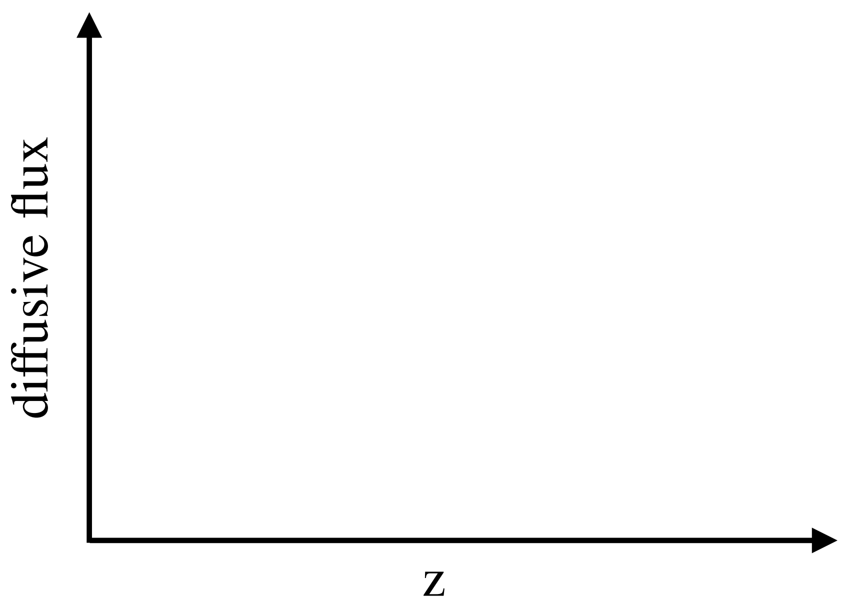
$$n_1 = j_1 + c_1 v^v$$

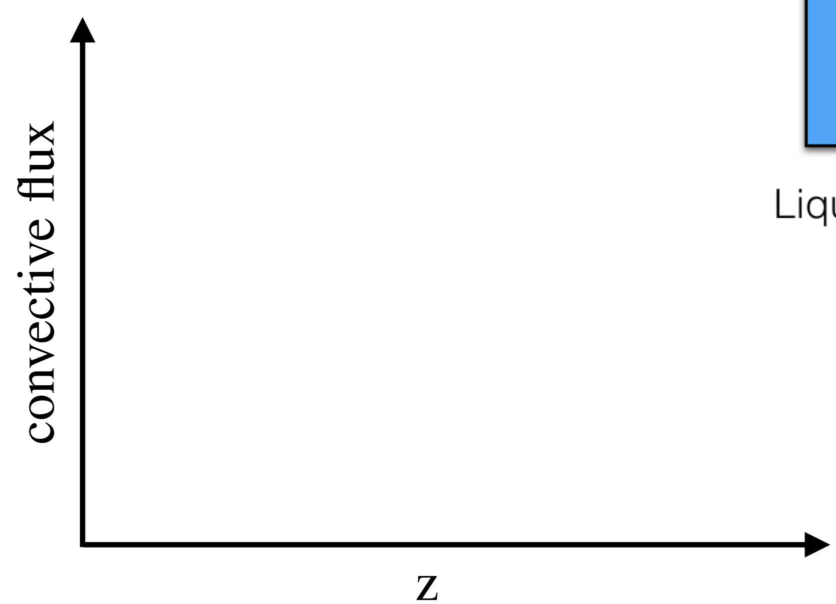
$$n_1 = \frac{D\bar{c}}{l} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

$$v^v = c_1 \bar{V}_1 v_1 = \bar{V}_1 n_1 \textbf{ (constant)}$$



Liquid evaporation through a capillary



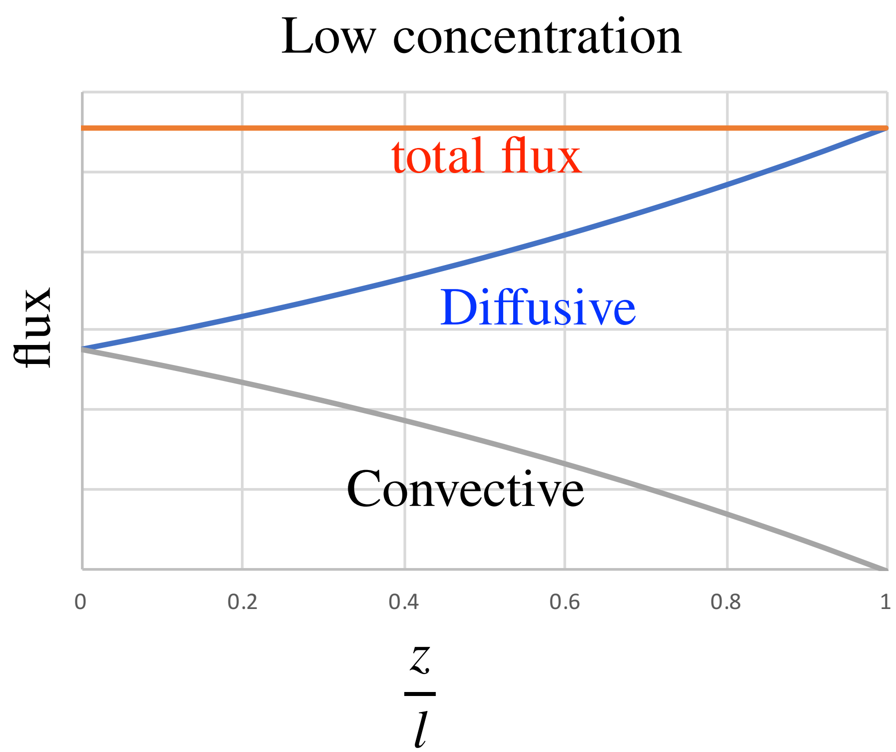


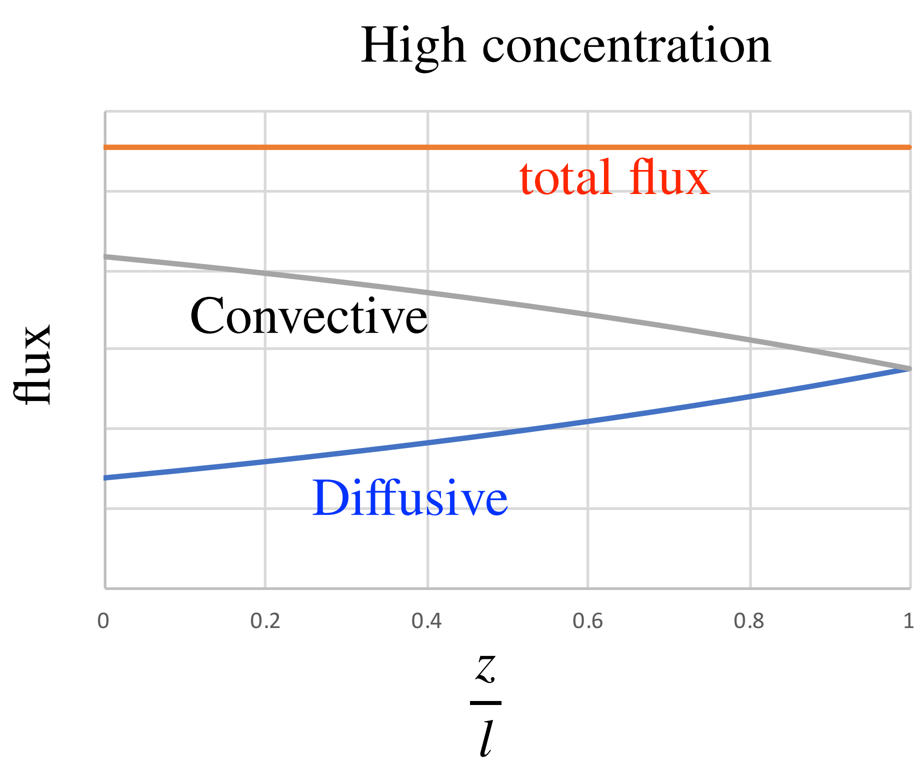
$$n_1 = -D\frac{dc_1}{dz} + c_1 v^v$$

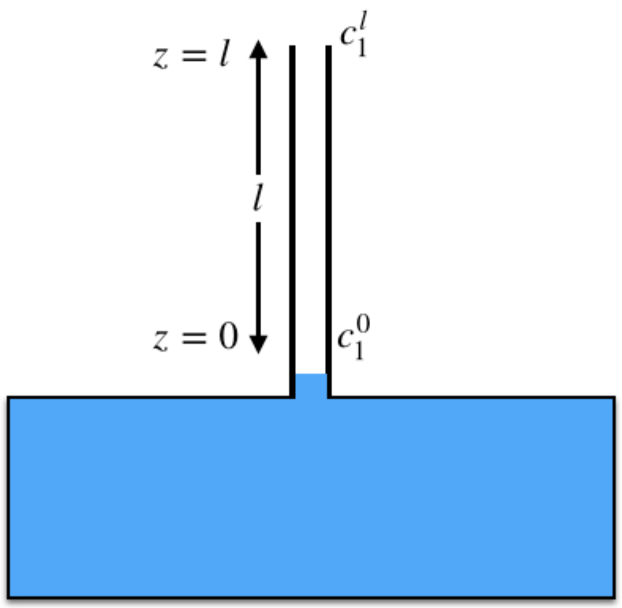
$$v^v = c_1 \bar{V}_1 v_1 = \bar{V}_1 n_1 \textbf{ (constant)}$$

Convection is higher at higher concentration

Relative contribution of diffusion and convection







Liquid evaporation through a capillary

Relative contribution of diffusion and convection

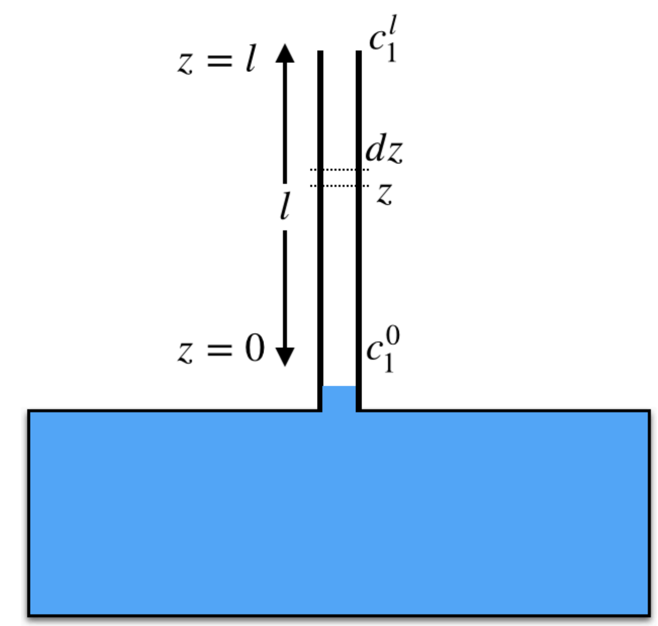
$$n_1 = j_1 \ + \ c_1 v^v \qquad n_1 \ = \ \frac{D\bar{c}}{l} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right) \qquad \frac{\bar{c} - c_1}{\bar{c} - c_1^0} \ = \ \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}}$$

Diffusive part

$$j_1 = -D\frac{dc_1}{dz}$$

Derivative of concentration profile (LHS)

$$\frac{d}{dz}\left(\frac{\bar{c} - c_1}{\bar{c} - c_1^0}\right) = -\left(\frac{1}{\bar{c} - c_1^0}\right)\frac{dc_1}{dz}$$



Liquid evaporation through a capillary

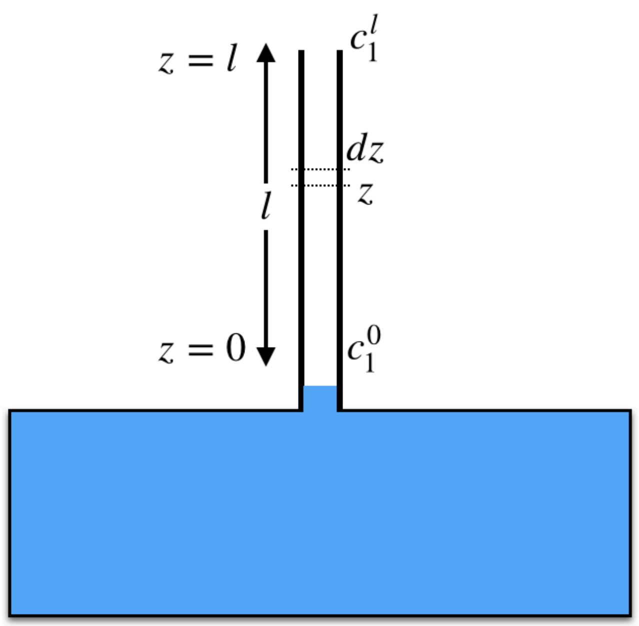
Derivative of RHS

$$\frac{da^z}{dz} \ = \ a^z \ln a$$

$$\frac{d}{dz}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} = \frac{1}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

$$j_1 = -D\frac{dc_1}{dz} \ = \ \frac{D(\bar{c} - c_1^0)}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

Alternatively



Liquid evaporation through a capillary

Convective flux

$$c_1 v^v = c_1 \bar{V}_1 n_1 = \frac{c_1}{\bar{c}} n_1 \approx y_1 n_1$$

Diffusive flux = Total flux - Convective flux

$$j_1 = n_1 - c_1 v^v = n_1 - \frac{c_1}{\bar{c}} n_1 = n_1 \left(\frac{\bar{c} - c_1}{\bar{c}} \right)$$

$$n_1 = \frac{D\bar{c}}{l} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right)$$

$$\Rightarrow j_1 = \frac{D\bar{c}}{l} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right) \left(\frac{\bar{c} - c_1}{\bar{c}} \right)$$

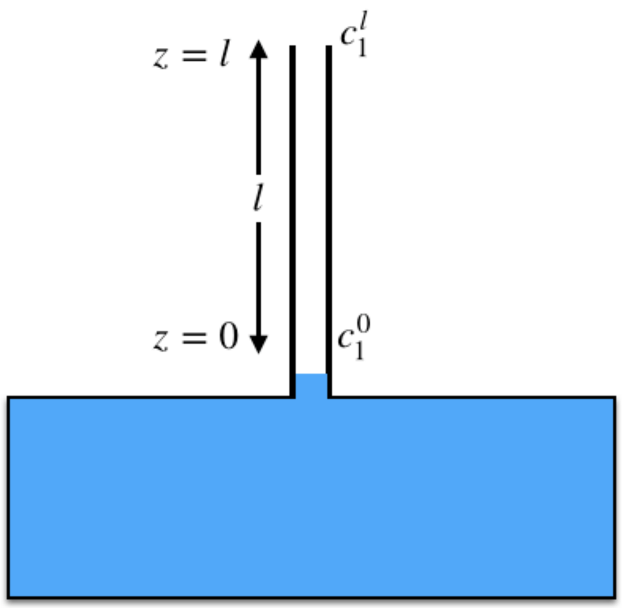
$$\frac{\bar{c} - c_1}{\bar{c} - c_1^0} = \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right)^{\frac{z}{l}} \longrightarrow (\bar{c} - c_1) = (\bar{c} - c_1^0) \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right)^{\frac{z}{l}}$$

$$\Rightarrow j_1 = \frac{D(\bar{c} - c_1^0)}{l} \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right)^{\frac{z}{l}} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0} \right)$$

Relative contribution of diffusion and convection

Total flux is constant $$n_1 = \frac{D\bar{c}}{l}\ln\left(\frac{\bar{c}-c_1^l}{\bar{c}-c_1^0}\right)$$

$$j_1 = \frac{D(\bar{c}-c_1^0)}{l}\left(\frac{\bar{c}-c_1^l}{\bar{c}-c_1^0}\right)^{\frac{z}{l}}\ln\left(\frac{\bar{c}-c_1^l}{\bar{c}-c_1^0}\right)$$



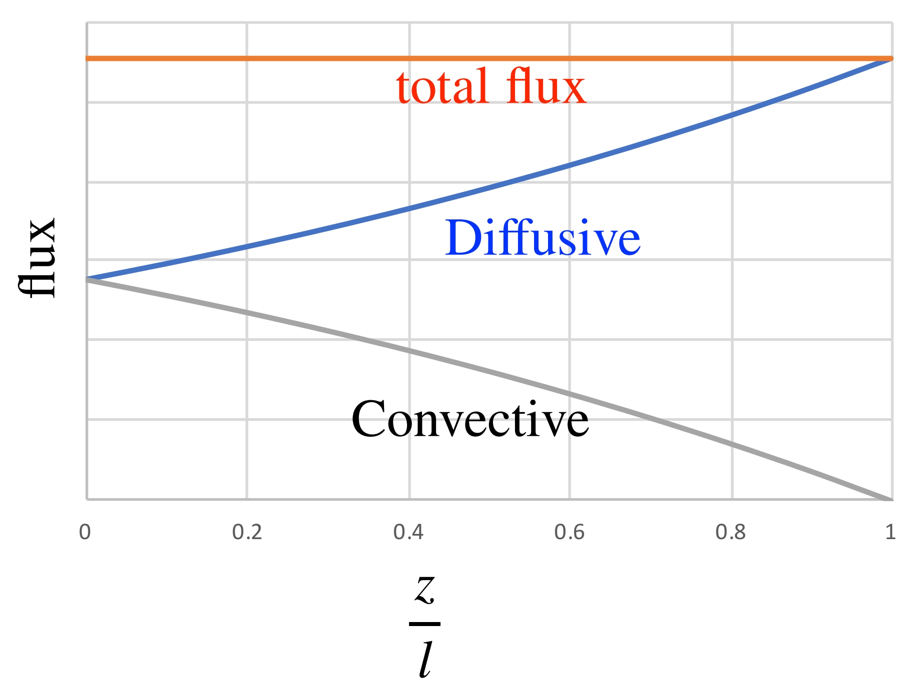
Liquid evaporation through a capillary

$\left(\frac{\bar{c}-c_1^l}{\bar{c}-c_1^0}\right) > 1 \Rightarrow$ **Diffusive part is maximum at $z = l$**

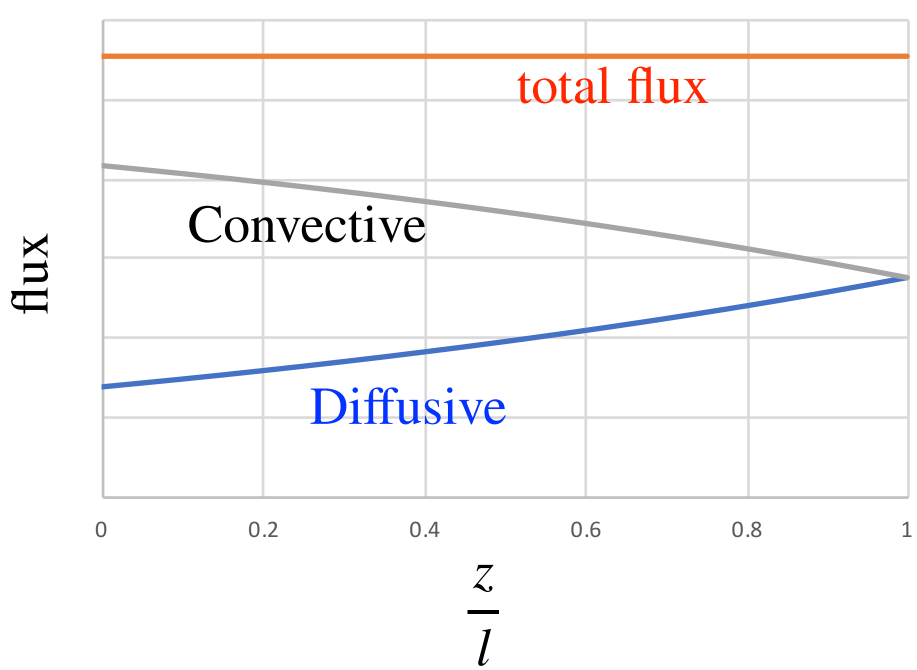
Convective part $= n_1 - j_1 = \frac{c_1}{\bar{c}} n_1$ is maximum at $z = 0$

- **Higher concentration c_1^0 leads to higher total flux**

Low concentration



High concentration

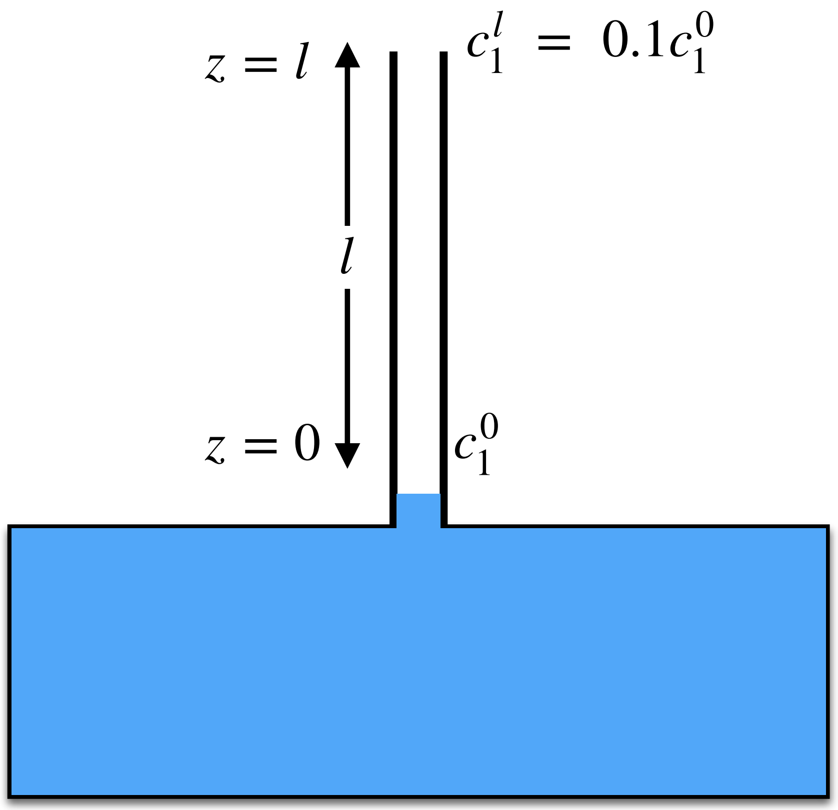


In class problem:

Calculate velocity of component 1 at z = 0 and z = l

$$c_1^0 = 0.02 \text{ mole/liter} \qquad c_1^l = 0.1 c_1^0$$

$$D = 1 \text{ cm}^2 \text{ s}^{-1} \qquad l = 10 \text{ cm}$$



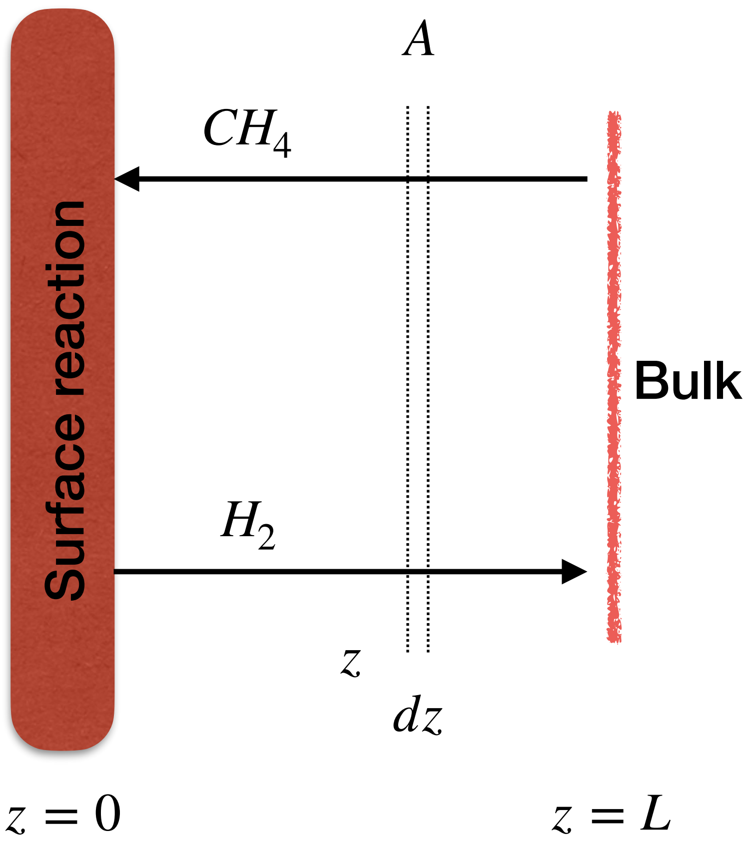
Liquid evaporation through a capillary

EPFL

Consider the following problem with diffusion, convection and reaction at steady-state

$$CH_4 \rightarrow C + 2H_2$$

Calculate concentration profile of CH_4



$C_{CH_4} = c_1^0 = 0$ $\quad$ $C_{CH_4} = c_1^L$

Define your system -

Define an element to do mass balance

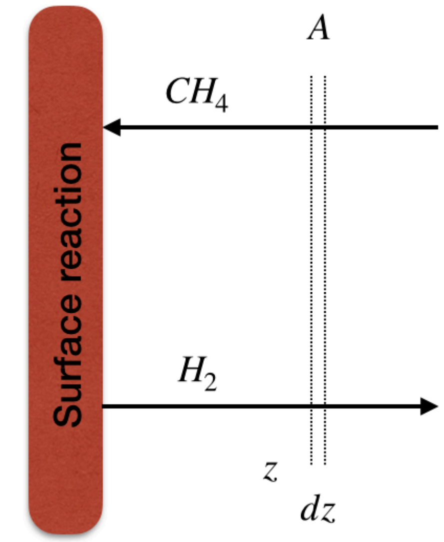
Apply mass balance

$$Accum\overset{o}{u}lation * dV = Fl\overset{o}{u}x|_{in} * A - Fl\overset{o}{u}x|_{out} * A + Gene\overset{o}{r}ation * dV - Consu\overset{o}{m}ption * dV$$

$$\frac{dn_1}{dz} = 0$$ n_1 is constant

Similarly

$$\frac{dn_2}{dz} = 0$$ n_2 is constant



Let's look at the boundary; z = 0

$$CH_4 \rightarrow C + 2H_2 \qquad n_2 = -2n_1 \qquad n = n_1 + n_2 = n_1 - 2n_1 = -n_1$$

We can use mole average velocity because we are dealing with gases

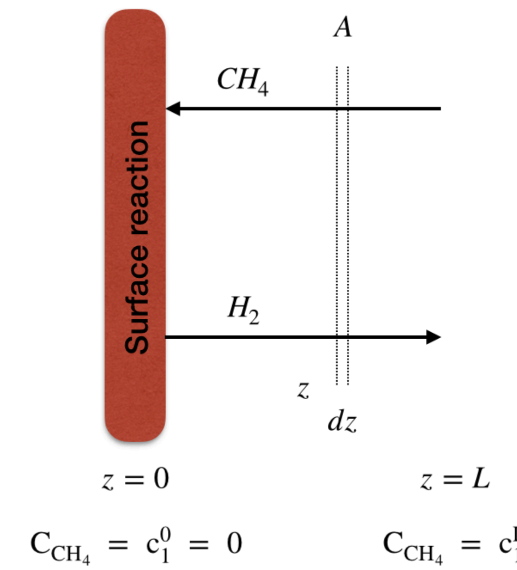
$$v = y_1 v_1 + y_2 v_2 \qquad n_1 = -Dc\nabla y_1 + c_1 v \qquad n = n_1 + n_2 = cv$$

$$\Rightarrow \quad n_1 = -Dc\nabla y_1 + y_1 cv$$

$$\Rightarrow \quad n_1 = -Dc\nabla y_1 + y_1 n \qquad n_1(1 + y_1) = -Dc\frac{dy}{dz}$$

$$\Rightarrow \quad n_1 = -Dc\nabla y_1 - y_1 n_1 \qquad \int_0^z \frac{n_1}{Dc}dz = -\int_0^{y_1} \frac{dy}{(1 + y_1)} \qquad at\ z = 0,\ C_{CH_4} = c_1^0 = 0$$

$$\int_0^z \frac{n_1}{Dc} dz = -\int_0^{y_1} \frac{dy}{(1+y_1)}$$



$$\Rightarrow \frac{n_1 z}{Dc} = -\ln(1+y_1)$$

$at\ z = L,\ C_{CH_4} = c_1^L$

$$\Rightarrow \frac{n_1 L}{Dc} = -\ln(1+y_1^L) \qquad \Rightarrow n_1 = -\frac{Dc}{L}\ln(1+y_1^L)$$

$$\Rightarrow \ln(1+y_1) = -\frac{n_1 z}{Dc} = \frac{z}{L}\ln(1+y_1^L) = \ln(1+y_1^L)^{z/L}$$

$$\Rightarrow 1+y_1 = (1+y_1^L)^{z/L}$$

$$\Rightarrow y_1 = (1+y_1^L)^{z/L} - 1$$

Exercise problem #1

Compare total flux when you consider convection and when you neglect convection (use thin film result without convection)

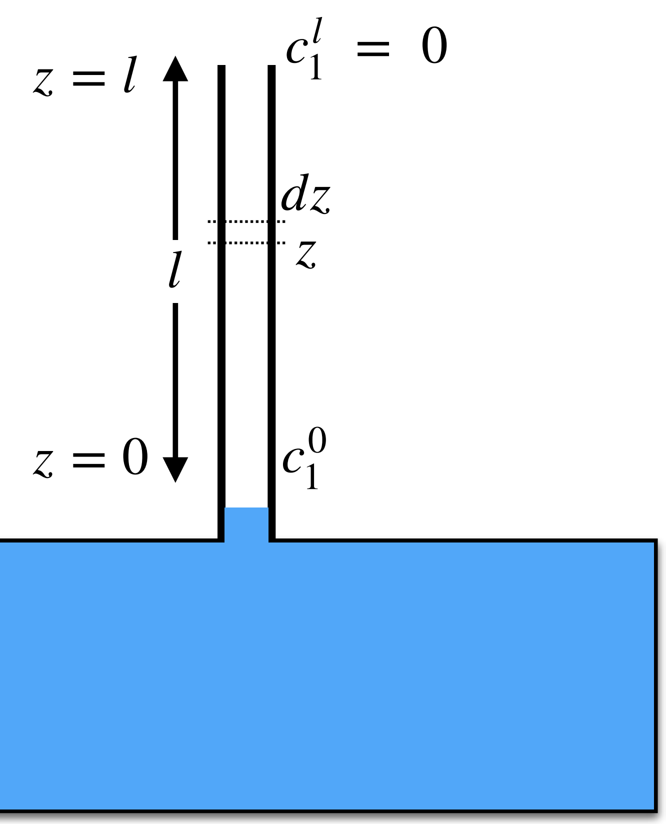
Consider two cases (stagnant air):

Benzene evaporating at 6 °C and 78 °C, Total pressure = 1 atm

$c_1^l = 0$ **D = 0.01 cm²/s; l = 1 m**

$$\bar{c} = \frac{P}{RT} \qquad c_1^0 = \frac{P^{sat}}{RT}$$

T (°C)	P^{sat} (atm)
6	0.049
78	0.934



Liquid evaporation through a capillary

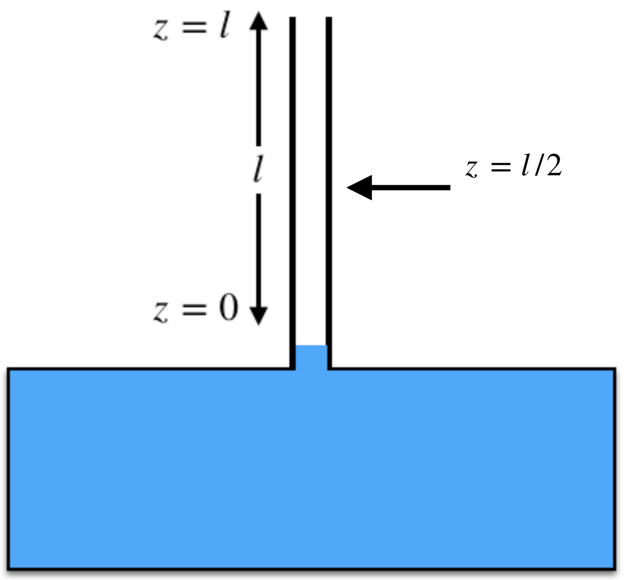
T (°C)	P^{sat}	$P \ln\left(\frac{P}{P - P^{sat}}\right)$	% Convection
6	0.049		
78	0.934		

Exercise problem #2

We said the air was stagnant, can you calculate the diffusive and convective flux of air?

$$v_2 = 0 \qquad \Rightarrow n_2 = c_2 v_2 = 0$$

$$n_2 = j_2 + c_2 v^v \qquad \Rightarrow j_2 = -c_2 v^v$$



Liquid evaporation through a capillary

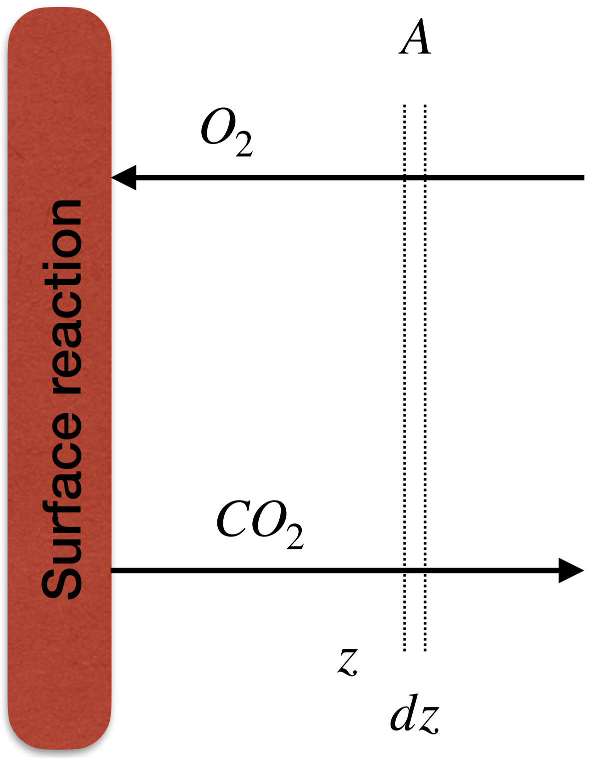
Average velocity of volume = v^v

Exercise problem #3

$$C + O_2 \;\rightarrow\; CO_2$$

Calculate concentration profile of O_2

Calculate velocity of CO_2 at $z = L$



$z = 0$ $\qquad$ $z = L$

$c_1^0 = c_1^L/10$ $\qquad$ $C_{O_2} = c_1^L$

$C_{CO_2} = c_2^L$