ChE-402: Diffusion and Mass Transfer

Lecture 4

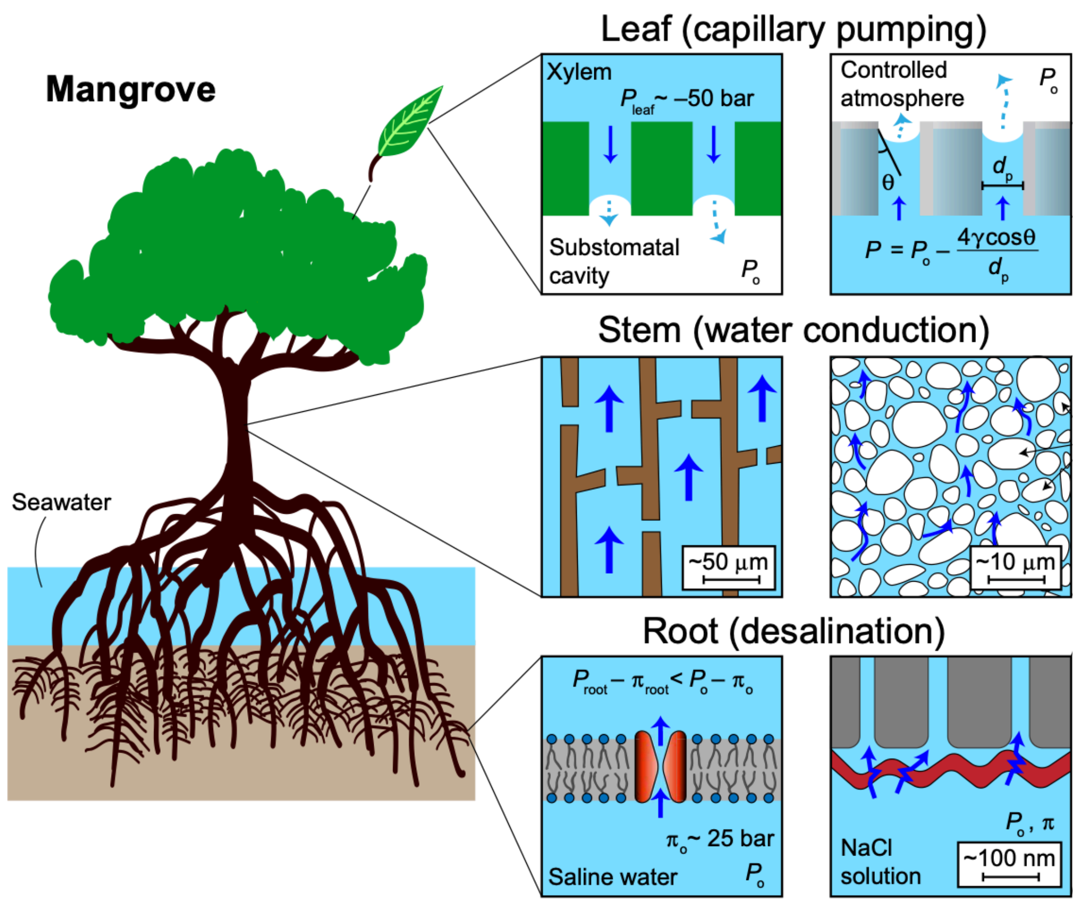
A train is running at a velocity of 100 km/h. It is crowded and carrying people who are moving around. Density of people ~ 1 person/m2. Calculate convective flux

A. Not enough information
B. 0
C. Convective flux is 100 * 1
D. It depends on diffusive flux

Intended Learning Outcome

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

Capillary evaporation

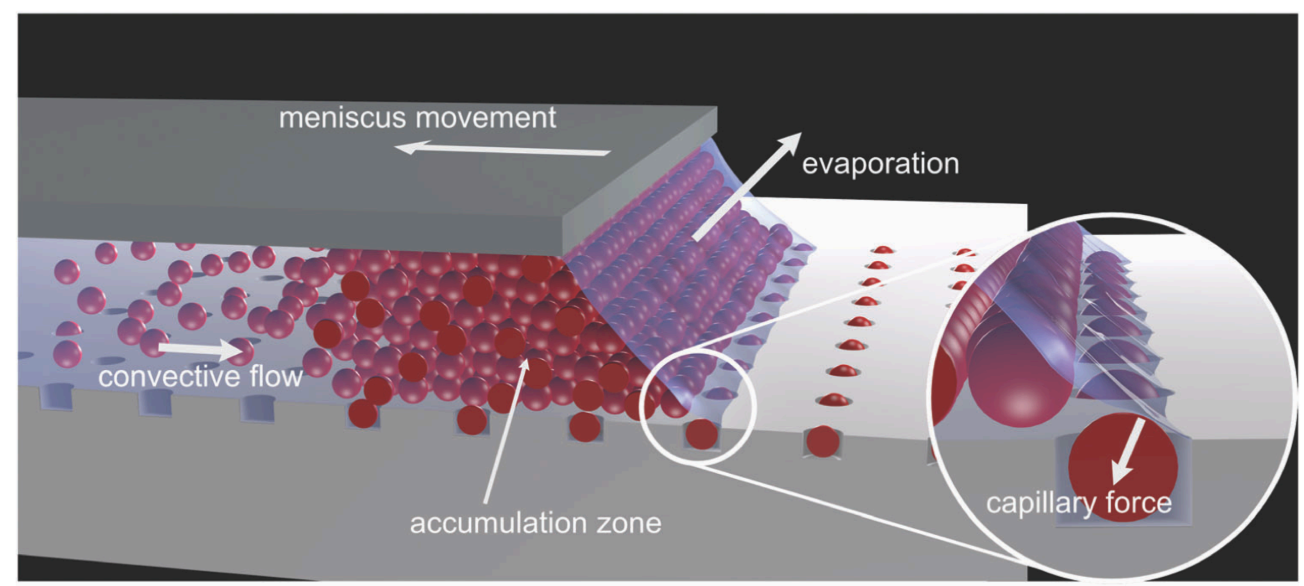


SCIENCE ADVANCES | RESEARCH ARTICLE

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

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

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

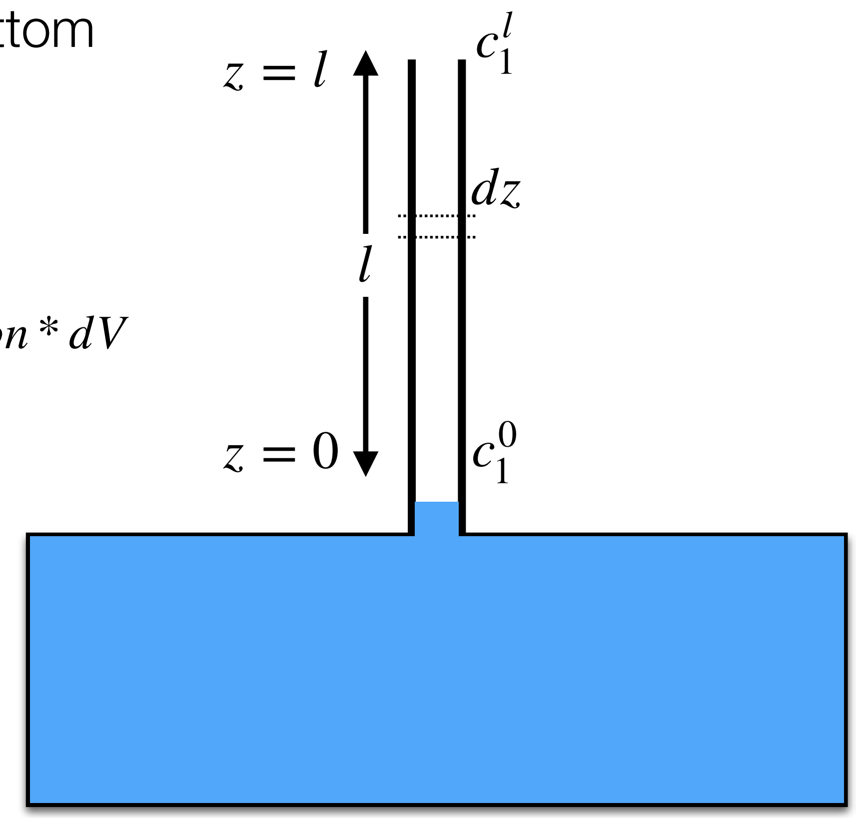
Solving the evaporation problem in stagnant air

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: dz at a distance z from bottom



Liquid evaporation through a capillary

Apply mass balance

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

$$0 \;\; (steady-state) = A\;(j_1^a + c_1 v^a)\;|_z - A\;(j_1^a + c_1 v^a)\;|_{z+dz} + 0 - 0$$

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

$$0 \; = \; A\; n_1\;|_z - A\; n_1\;|_{z+dz}$$

$$\frac{dn_1}{dz} \; = \; 0$$

n_1 is constant

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

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

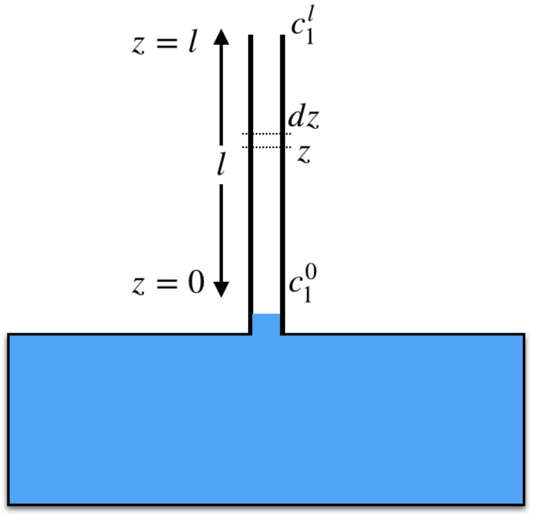
$\bar{V}_1 = \bar{V}_2 = \frac{1}{\bar{c}}$ is constant (e.g., 22.4 liter/mole in vapor phase at STP)

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

$z = 0; \quad c_1 = c_1^0$ (saturated vapor at equilibrium)

$z = l; \quad c_1 = c_1^l$

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



Liquid evaporation through a capillary

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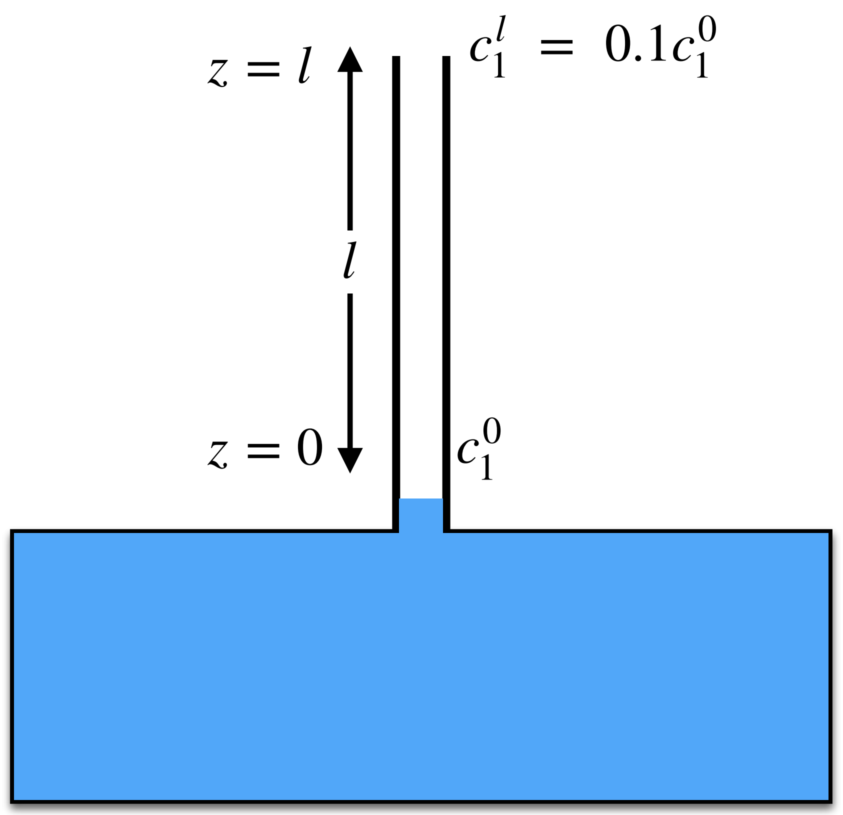
Where is the velocity maximum in this case

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



Liquid evaporation through a capillary

$$v_1 = \frac{n_1}{c_1}$$

n_1 is constant; c_1 is highest at $z = 0$ and lowest at $z = l$

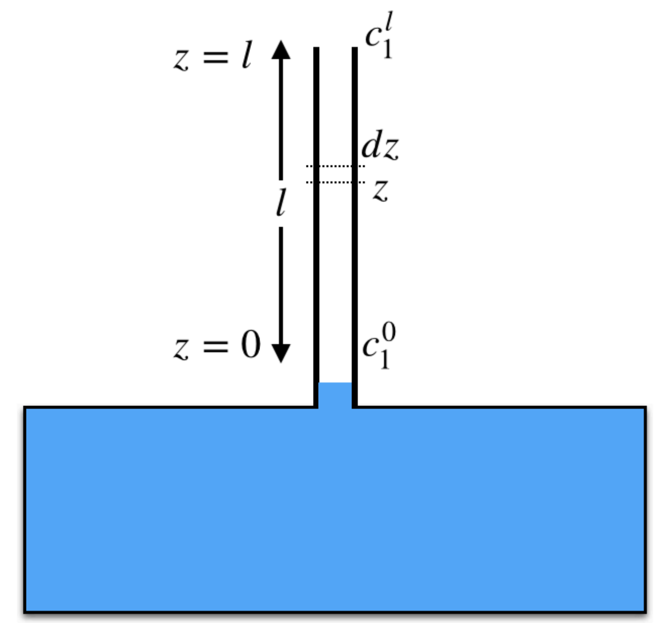
So, velocity is highest at $z = l$

Relative contribution of diffusion and convection

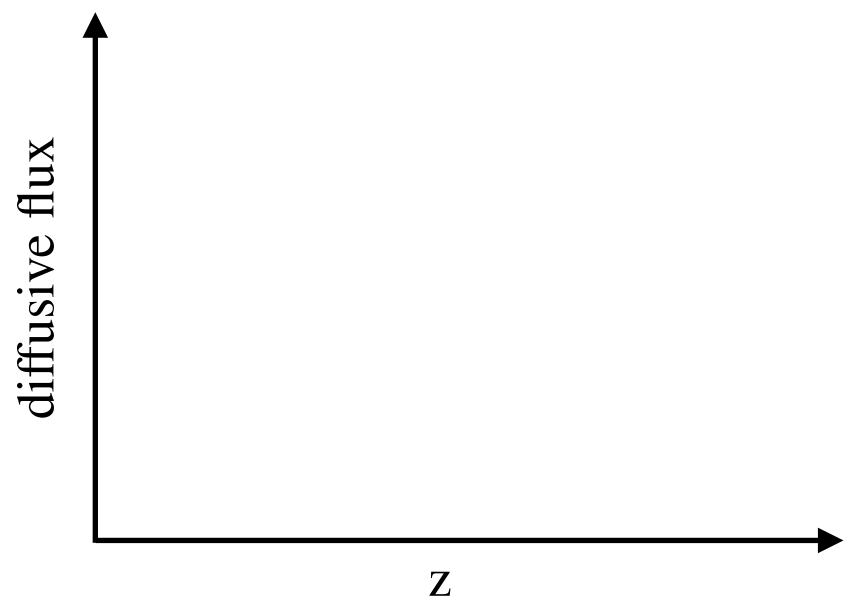
$$n_1 = j_1 + c_1 v^v$$

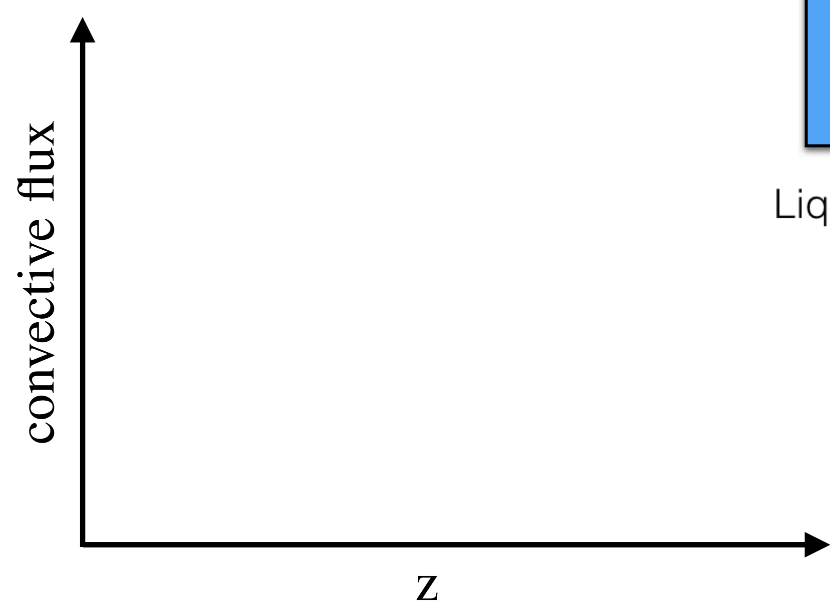
$$n_1 = \frac{D\bar{c}}{l} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

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



Liquid evaporation through a capillary



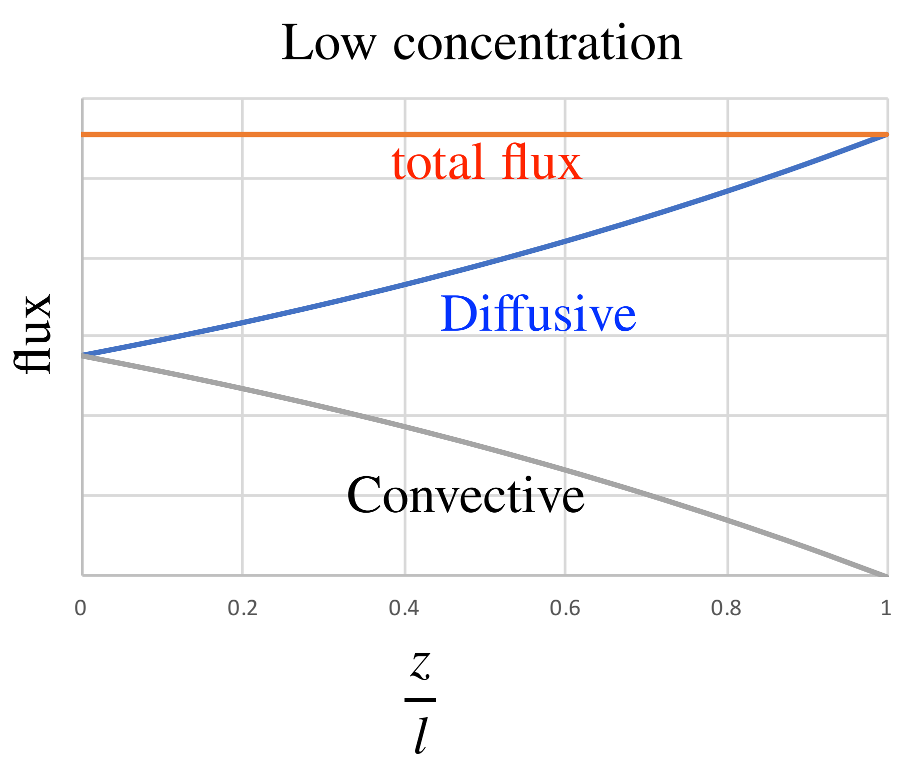


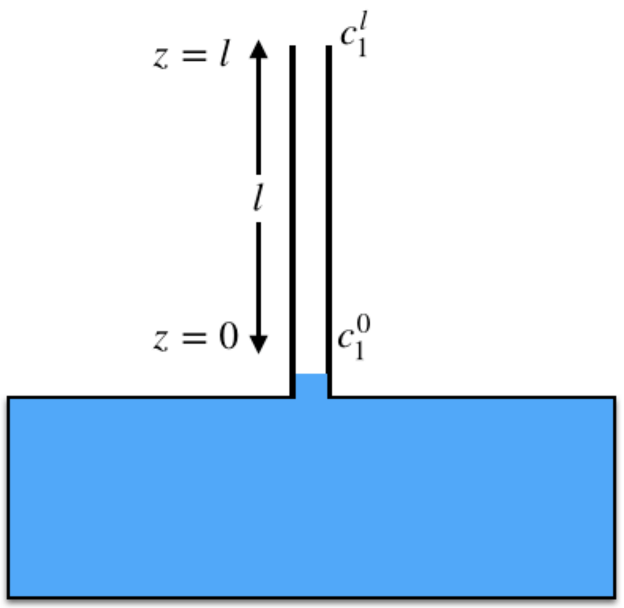
$$n_1 = -D\frac{dc_1}{dz} + c_1 v^v$$

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

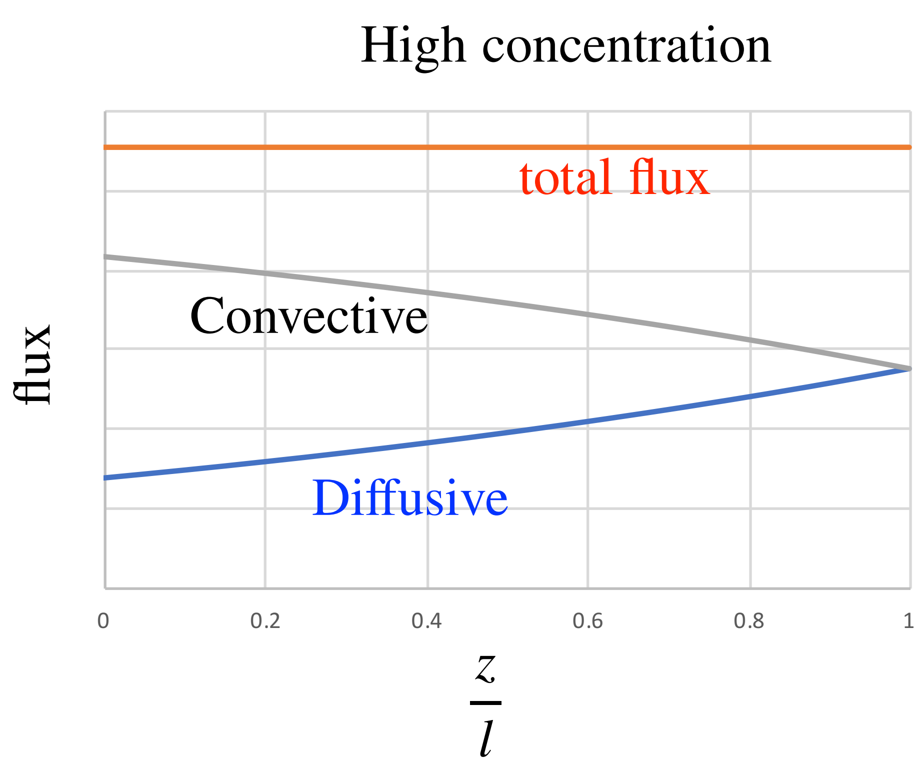
Convection is higher at higher concentration

Relative contribution of diffusion and convection





Liquid evaporation through a capillary



Relative contribution of diffusion and convection

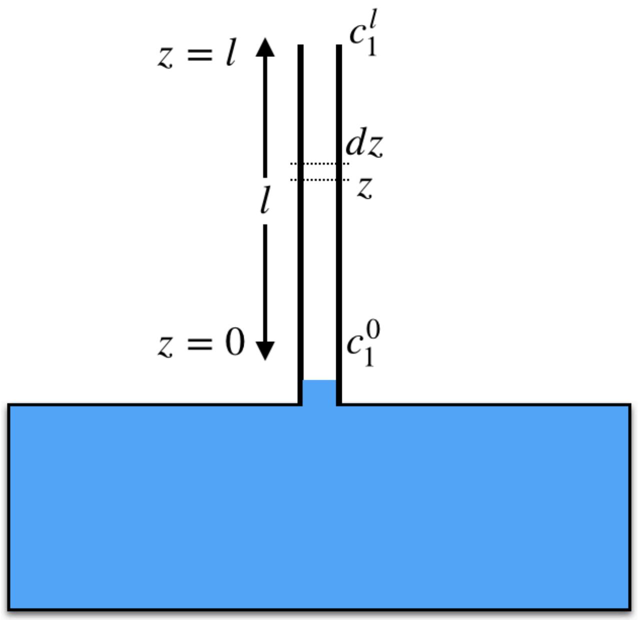
$$n_1 = j_1 + c_1 v^v \qquad n_1 = \frac{D\bar{c}}{l}\ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right) \qquad \frac{\bar{c} - c_1}{\bar{c} - c_1^0} = \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}}$$

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

$$\frac{da^z}{dz} = a^z \ln a \qquad a = \left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right) \qquad \Rightarrow -\left(\frac{1}{\bar{c} - c_1^0}\right)\frac{dc_1}{dz} = \frac{1}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}}\ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

$$\frac{d}{dz}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} = \frac{1}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}}\ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right) \qquad j_1 = -D\frac{dc_1}{dz} = \frac{D(\bar{c} - c_1^0)}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}}\ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$

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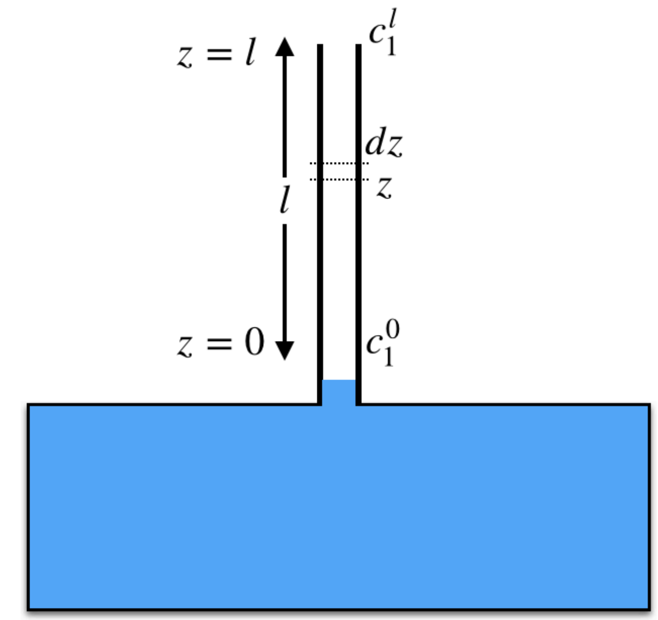
Alternatively



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

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

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

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

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

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

EPFL

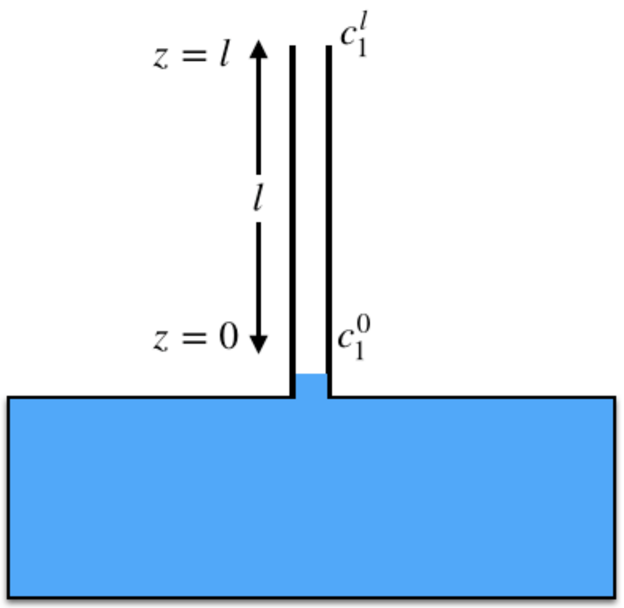
Relative contribution of diffusion and convection

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

$$j_1 = \frac{D(\bar{c} - c_1^0)}{l}\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)^{\frac{z}{l}} \ln\left(\frac{\bar{c} - c_1^l}{\bar{c} - c_1^0}\right)$$ Diffusive flux is not constant

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

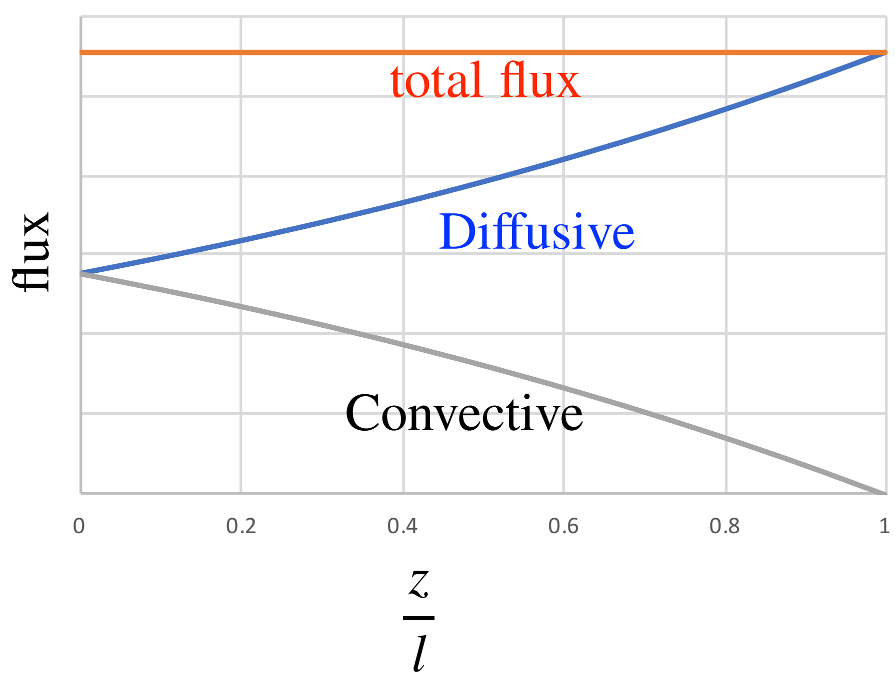
Convective part $= n_1 - j_1 = \frac{c_1}{\bar{c}} n_1$ is maximum at $z = 0$



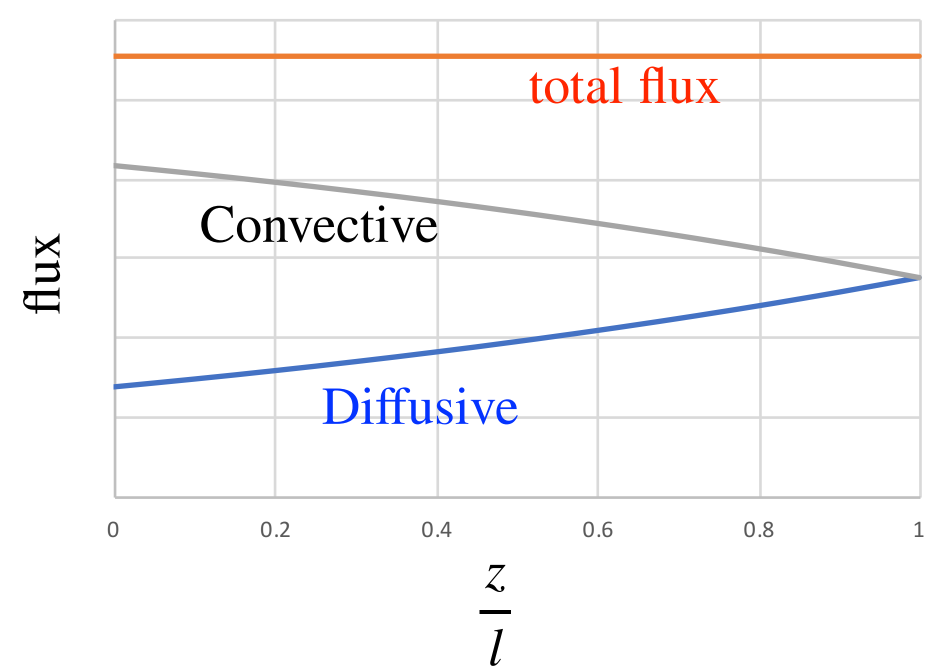
Liquid evaporation through a capillary

- **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 $z = l$

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

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

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

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

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

$$\bar{c} = 0.045 \text{ mole/liter}$$

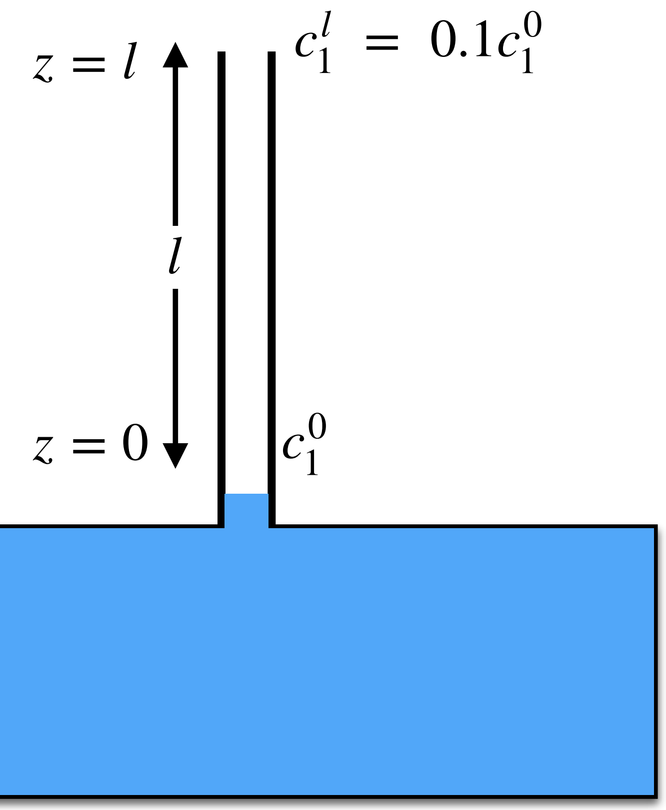
$$\text{velocity of component 1} = \mathrm{v}_1 = \frac{\mathrm{n}_1}{\mathrm{c}_1}$$

$$n_1 = \frac{10^{-4} * 0.045 * 1000}{0.1} \ln\left(\frac{0.045 - 0.002}{0.045 - 0.02}\right)$$

$$= 2.44 * 10^{-2} \text{ mole m}^{-2} \text{ s}^{-1}$$

$$v_1^0 = \frac{2.44 * 10^{-2}}{0.02 * 1000} = 1.22 * 10^{-3}\ m\ s^{-1}$$

$$v_1^l = \frac{2.44 * 10^{-2}}{0.002 * 1000} = 1.22 * 10^{-2}\ m\ s^{-1}$$



Liquid evaporation through a capillary

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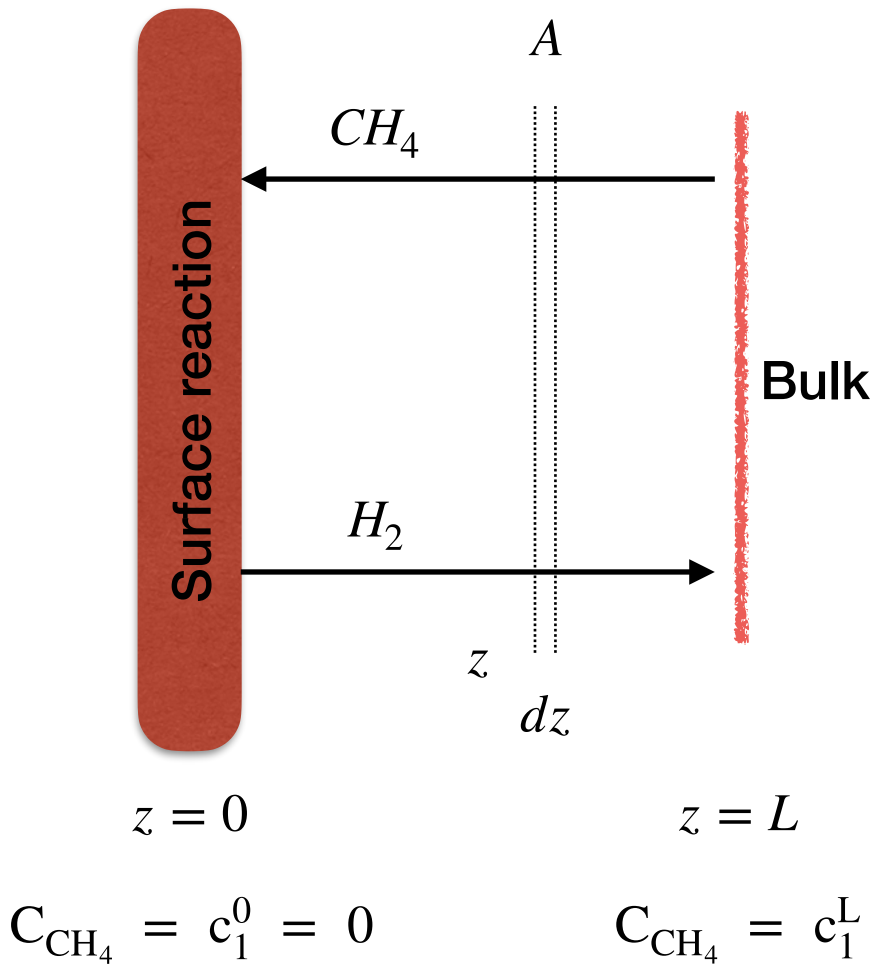
Consider the following problem with diffusion, convection and reaction at steady-state

$$CH_4 \rightarrow C + 2H_2$$

Calculate concentration profile of CH_4



Define your system - Space from z = 0 to z= L

Define an element to do mass balance

Apply mass balance

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

$$0 \ \ (steady-state) = A \ n_1 \,|_z - A \ n_1 \,|_{z+dz} + 0 - 0$$

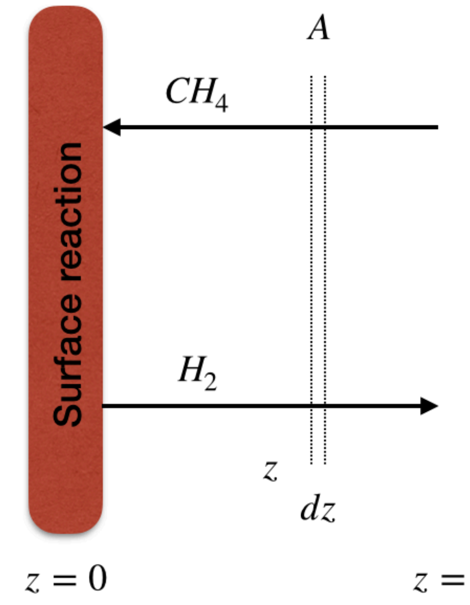
$$\frac{dn_1}{dz} = 0$$

n_1 is constant

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

Similarly

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



$z = 0$ $C_{CH_4} = c_1^0 = 0$

$z = L$ $C_{CH_4} = c_1^L$

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

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

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

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

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

$$at\ z = 0, \; C_{CH_4} = c_1^0 = 0$$

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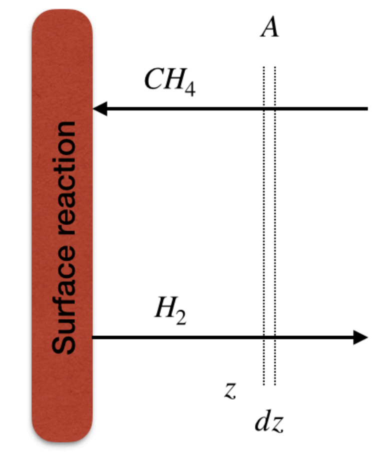
$$\int_0^z \frac{n_1}{Dc} dz = -\int_0^{y_1} \frac{dy}{(1+y_1)}$$



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

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

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

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

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

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

EPFL