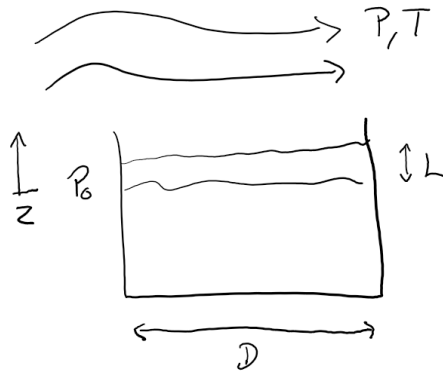


1)



$$P = 101325 \text{ Pa}$$

$$T = 25 \text{ }^{\circ}\text{C}$$

$$L = 0.50 \text{ in} = 0.0127 \text{ m}$$

$$D = 15 \text{ ft} = 4.572 \text{ m}$$

$$D_{AB} = 0.08 \times 10^{-4} \text{ m}^2/\text{s}$$

$$\gamma_B (65 \text{ }^{\circ}\text{F}) = 0.875$$

$$P_B^{sat} = 105 \text{ mmHg}$$

**Assume:** A = Air, B = Benzene,  $P_{B,L} \approx 0$ , ideal gasses, benzene height is constant

**Solve:**

By Fick's first law, we have,

$$N_B = -\frac{PD_{AB}}{RT} \frac{dy_B}{dz} + y_B (N_A + N_B).$$

Since the air is assumed stagnant,  $N_A = 0$ , giving upon rearrangement,

$$N_B = -\frac{PD_{AB}}{RT} \frac{1}{1 - y_B} \frac{dy_B}{dz},$$

assuming steady state and integrating from  $z = 0$  to  $z = L$ ,

$$N_B = \frac{PD_{AB}}{RTL} \ln \left( \frac{1 - y_{B,L}}{1 - y_{B,0}} \right).$$

$y_{B,L} \approx 0$  and  $y_{B,0} = P_B^{sat}/P = 0.138$  based on our assumptions. The amount of benzene diffused from the tank is then given by integrating the flux over the evaporation area,

$$\dot{n}_B = \int_A N_B dA = -\frac{\pi D^2}{4L} \frac{PD_{AB}}{RT} \ln(1 - y_{B,0}),$$

or in mass flows,

$$\dot{m}_B = -\frac{\pi D^2}{4L} \frac{PM_B D_{AB}}{RT} \ln(1 - y_{B,0}).$$

Numerically,

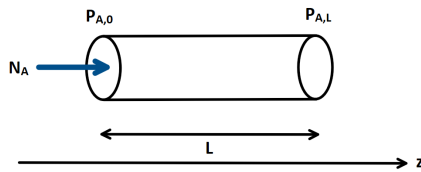
$$\begin{aligned} \dot{m}_B &= -\frac{\pi(4.572^2 \text{ m}^2)}{4(0.0127 \text{ m})} \frac{(101325 \text{ J/m}^3)(0.07811 \text{ kg/mol})(8 \times 10^{-6} \text{ m}^2/\text{s})}{(8.314 \text{ J/mol} \cdot \text{K})(298.15 \text{ K})} \ln(1 - 0.138) \\ &= 0.0049 \text{ kg/s.} \end{aligned}$$

Converting to lb/day,

$$\boxed{\dot{m}_B = 935 \text{ lb/day}}.$$

Using Antoine's equation <sup>1</sup>, the vapor pressure of benzene at the given temperature is 12.69 kPa and an experimental value of diffusivity <sup>2</sup> is given as  $D_{AB} = 0.077 \text{ cm}^2/\text{s}$ . Performing the same calculations with the updated value gives  $\dot{m}_B = 810 \text{ lb/day}$ , which is about 15% smaller. This is mainly because the updated  $P_B^{sat}$  is smaller, resulting in a smaller driving force and rate.

2)



$$P = 101325 \text{ Pa}$$

$$T = 25 \text{ }^\circ\text{C}$$

$$L = 1 \text{ m}$$

$$D = 1.049 \text{ in} = 0.0266 \text{ m}$$

$$D_{AB} = 0.694 \times 10^{-4} \text{ m}^2/\text{s}$$

$$P_{A,0} = 0.80 \text{ atm}$$

$$P_{A,L} = 0.10 \text{ atm}$$

**Assume:** A = H<sub>2</sub>, B = CH<sub>4</sub>, ideal gasses

**Solve:**

**a.**

From Fick's first law,

$$N_A = -\frac{PD_{AB}}{RT} \frac{dy_A}{dz} + y_A (N_A + N_B),$$

we assume there is no bulk flow and thus,  $N_A = -N_B$ . Integrating from  $z = 0$  to  $z = L$ ,

$$N_A = -\frac{PD_{AB}}{RT} \frac{y_{A,L} - y_{A,0}}{L}.$$

Numerically,

$$N_A = \frac{(101325 \text{ J/m}^3)(0.694 \times 10^{-4} \text{ m}^2/\text{s})}{(8.314 \text{ J/mol} \cdot \text{K})(298 \text{ K})} \frac{0.80 - 0.10}{1 \text{ m}} = 0.00199 \text{ mol}/(\text{m}^2 \cdot \text{s}).$$

<sup>1</sup>Smith, J.M., Van Ness, H.C., Abbot, M. M., Swihart, M. T., *Introduction to Chemical Engineering Thermodynamics*. 9th Ed., McGraw Hill, 2018.

<sup>2</sup>Perry, R.H., Green, D. W., Maloney, J.O., *Perry's Chemical Engineers' Handbook*, 7th ed., McGraw-Hill, 1997.

**b.**

By a material balance around a cross section of the pipe, the number of moles collected at the far end of the pipe is,

$$n_A = \int_0^t \int_A N_A dA dt.$$

If  $N_A$  is constant,

$$n_A = \frac{\pi D^2}{4} N_A t,$$

or,

$$t = \frac{4}{\pi D^2} \frac{n_A}{N_A}.$$

Numerically,

$$t = \frac{4}{\pi(0.0266^2 \text{ m}^2)} \frac{20 \text{ mol}}{0.00199 \text{ mol}/(\text{m}^2 \cdot \text{s})} = 18054018 \text{ s},$$

$$\implies \boxed{t = 209 \text{ days}}.$$

**c.**

The material balance in integral form is,

$$\int_V \left( \frac{\partial c_A}{\partial t} + \frac{\partial N_A}{\partial z} \right) dV = 0,$$

with Fick's law,

$$\frac{\partial c_A}{\partial t} - D_{AB} \frac{\partial^2 c_A}{\partial z^2} = 0,$$

with initial and boundary conditions (assuming the concentration profile starts out flat),

$$c_A(0, t) = c_{A,0}, \quad c_A(L, t) = c_{A,L}, \quad c_A(z, 0) = c_{A,L}.$$

Define a new variable,  $C$ , as,

$$C = c_A - \left[ c_{A,0} + (c_{A,L} - c_{A,0}) \frac{z}{L} \right],$$

plugging this into the original PDE,

$$\frac{\partial C}{\partial t} - D_{AB} \frac{\partial^2 C}{\partial z^2} = 0,$$

with initial and boundary conditions,

$$C(0, t) = 0, \quad C(L, t) = 0, \quad C(z, 0) = (c_{A,L} - c_{A,0}) \left[ 1 - \frac{z}{L} \right].$$

I remember solving this in my PDE class - not a fun equation to solve. I have dug up the solution here,

$$c_A(z, t) = \left[ c_{A,0} + (c_{A,L} - c_{A,0}) \frac{z}{L} \right] + (c_{A,L} - c_{A,0}) \sum_{n=1}^{\infty} \frac{2}{n\pi} (1 - \cos(n\pi)) e^{-(\frac{n\pi}{L})^2 D t} \sin\left(\frac{n\pi z}{L}\right),$$

The flux is then given by taking the derivative,

$$N_A(z, t) = D_{AB} (c_{A,0} - c_{A,L}) \left[ \frac{1}{L} + \sum_{n=1}^{\infty} \frac{2}{L} (1 - \cos(n\pi)) e^{-(\frac{n\pi}{L})^2 D_{AB} t} \cos\left(\frac{n\pi z}{L}\right) \right],$$

Integrating over the pipe area and time,

$$n_A(z) = \frac{\pi D^2}{4} D_{AB} \left( \frac{c_{A,0} - c_{A,L}}{L} \right) \left[ t - \sum_{n=1}^{\infty} \frac{2e^{-(\frac{n\pi}{L})^2 D_{AB} t}}{(\frac{n\pi}{L})^2 D_{AB}} (1 - \cos(n\pi)) \cos\left(\frac{n\pi z}{L}\right) \right].$$

Looking carefully, the first term in the brackets is the steady state solution while the series offers corrections to account for spatial and temporal dependence of the flux. In practice, the diffusion time is so long that all of the series terms are essentially zero and the corrected solution is the same as the steady profile solution in part b.

Perhaps a more realistic boundary condition would be to just let the  $H_2$  naturally pass the end of the pipe rather than keep a fixed concentration. This condition can be approximated if we take the limit where  $L \rightarrow \infty$ <sup>3</sup>, which enables the use of Laplace transforms. This gives a new PDE,

$$\frac{\partial C}{\partial t} - D_{AB} \frac{\partial^2 C}{\partial z^2} = 0,$$

with,

$$C = \frac{c_A - c_{A,\infty}}{c_{A,0} - c_{A,\infty}},$$

and,

$$C(0, t) = 1, \quad C(\infty, t) = 0, \quad C(z, 0) = 0.$$

This is the heat equation in a semi-infinite medium, which has a 'well-known' solution,

$$C(z, t) = 1 - \frac{2}{\sqrt{\pi}} \int_0^\xi \exp(-x^2) dx,$$

where,

$$\xi = \frac{z}{\sqrt{4D_{AB}t}}.$$

The flux is then given by taking the derivative,

$$N_A(z, t) = (c_{A,0} - c_{A,\infty}) \sqrt{\frac{D_{AB}}{\pi t}} \exp\left(-\frac{z^2}{4D_{AB}t}\right).$$

The total moles passed through the far endpoint,  $L$ , is given by integrating over the pipe area and time,

$$n_A = \int_0^t \int_A N_A(L, t) dA dt = \frac{\pi D^2}{4} (c_{A,0} - c_{A,\infty}) \int_0^t \sqrt{\frac{D_{AB}}{\pi t}} \exp\left(-\frac{L^2}{4D_{AB}t}\right) dt.$$

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<sup>3</sup>Based on the long timescale from the previous question, this is a reasonable approximation.

This can be evaluated numerically to give,  $t = 563$  years. This is much longer since the  $\text{H}_2$  concentration continually increases at  $z = L$  and thus, less and less flux passes as the gradient becomes very small.

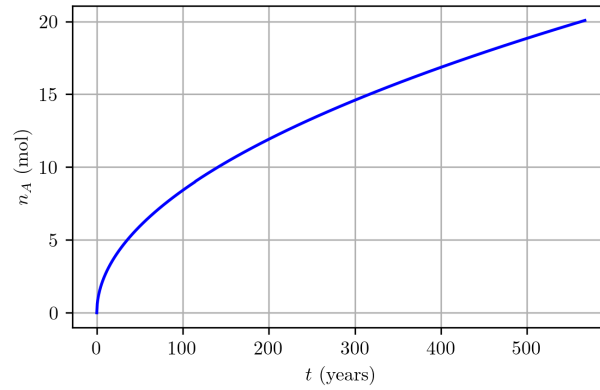


Figure 1: Moles collected at  $z = L$  over time