The University of Calgary
Department of Chemical & Petroleum Engineering

ENCH 501: Mathematical Methods in Chemical Engineering
Quiz #5

Time Allowed: 50 mins. **November 6, 2001**

Jeje

Dimethyl sulfoxide (DMSO) has many uses. Some restaurants soak cut lettuce and vegetables in dilute solutions to keep the "greens" crisp and "fresh" all day. Professional athletes also apply the solution topically (i.e. on the skin) as an analgesic (medication that reduces or eliminates pain) and an anti-inflammatory agent. It is the latter use that is of interest. Because an excess of the compound in the skin can cause irritation, itching and other discomforts, it is necessary to limit exposure of the skin to the compound and to restrict the amount of DMSO absorbed.

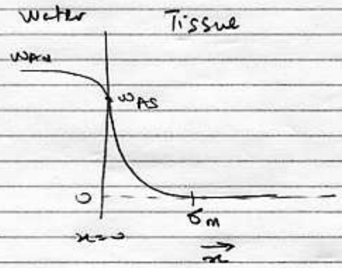
Consider that a swimming pool contains 2% mass basis DMSO in water. At $t = 0$ an athlete jumps in. We focus on his back and note that at the beginning there was no DMSO in the athlete's back skin. Because of his movement and the currents, the mass transfer coefficient in the liquid next to the skin, k_L, is determined to be $0.121\ cm/s$. The diffusivity of DMSO in skin is $2(10^{-9})\ m^2/s$ and the skin density is $1035\ kg/m^3$. The density of water is $1000\ kg/m^3$. Assume the skin is a homogeneous tissue and only DMSO is diffusing through the tissue.

Use the integral method to:

a) **(10 points)**
Derive a relationship between mass fraction of DMSO in tissue (ω_A), position and time.

b) **(Bonus 2 points)**
Estimate the amount of DMSO absorbed per unit area of the back skin in 30 minutes. Assume skin is semi-infinite.

ENCH 501 Solution to Quiz 5 Nov. 6, 2001



Integral method : — similar to heat transfer problem with convective b.c. in Notes.

Mass balance equation on domain

Input = Accumulation

$$n_A\Big|_{x=0} = \frac{d}{dt}\left[\int_0^{\delta_m} \rho_T w_A \, dx\right]$$

This is integral material balance eq.

Definition of mass flux in tissue

$$n_A = -\mathcal{D}_{AB}\rho_T \frac{\partial w_A}{\partial x} + w_A(n_A + \underbrace{\cancel{n_B}}_{\text{tissue stagnant}})$$

Re-arrange $n_A = -\dfrac{\mathcal{D}_{AB}\rho_T}{1-w_A}\dfrac{\partial w_A}{\partial x}$

At the boundary

$$x=0 \qquad n_A\Big|_{x=0} = \frac{-\mathcal{D}_{AB}\rho_T}{1-w_{AS}}\frac{\partial w_A}{\partial x}\Big|_{x=0} \quad ; \text{ note denominator}$$

$$= k_L \rho_w (w_{A\infty} - w_{AS})$$

other b.c.

$$x = \delta_m \qquad w_A = 0$$

$$x = \delta_m \qquad \frac{\partial w_A}{\partial x} = 0$$

Assume a concentration profile within the tissue of the form

$$\frac{w_A}{w_{AS}} = A + B\left(\frac{x}{\delta_m}\right) + C\left(\frac{x}{\delta_m}\right)^2$$

with conditions $x=0$, $w_A = w_{AS}$; $x=\delta_m$, $w_A = 0$

$x=\delta_m$, $\partial w_A/\partial x = 0$

Substitute conditions $A = 1$, $B = -2$, $C = 1$

or $$\frac{\omega_A}{\omega_{AS}} = \left(1 - \frac{x}{\delta_m}\right)^2$$

Substitute into integral equation

$$k_L \rho_w (\omega_{A\infty} - \omega_{AS}) = \frac{d}{dt}\left[\int_0^{\delta_m} \rho_T \omega_{AS}\left(1 - \frac{x}{\delta_m}\right)^2 dx\right]$$

where both ω_{AS} and δ_m are functions of time.

$$k_L \rho_w (\omega_{A\infty} - \omega_{AS}) = \frac{d}{dt}\left[\rho_T \omega_{AS} \delta_m \int_0^1 (1-\eta)^2 d\eta\right] \; ; \; \eta = \frac{x}{\delta_m}$$

$$k_L \rho_w (\omega_{A\infty} - \omega_{AS}) = \frac{d}{dt}\left[\rho_T \omega_{AS} \frac{\delta_m}{3}\right] \quad (1)$$

From b.c. at $x = 0$

$$\left.\frac{\partial \omega_A}{\partial x}\right|_{x=0} = \omega_{AS}\left(-\frac{2}{\delta_m} + \frac{2x}{\delta_m^2}\right)\Bigg|_{x=0} = -\frac{2\omega_{AS}}{\delta_m}$$

Hence $$\frac{D_{AB}\rho_T}{1-\omega_{AS}}\left(\frac{2\omega_{AS}}{\delta_m}\right) = k_L \rho_w (\omega_{A\infty} - \omega_{AS}) \quad (2)$$

Equation (2) can be re-arranged for δ_m or ω_{AS} and substituted into eq. (1) and solved.

$$\frac{2 D_{AB}}{k_L}\frac{\rho_T}{\rho_w}\frac{\omega_{AS}}{(\omega_{A\infty} - \omega_{AS})(1-\omega_{AS})} = \delta_m$$

or if $\omega_{AS} < \omega_{A\infty} << 1$ which is a good approximation here

$$\gamma/\delta_m = \frac{2 D_{AB}}{k_L}\frac{\rho_T}{\rho_w}\frac{1}{\delta_m} = \frac{\omega_{A\infty} - \omega_{AS}}{\omega_{AS}} = \frac{\omega_{A\infty}}{\omega_{AS}} - 1 \quad (3)$$

Equation ① is

$$\cancel{k_L \rho_W} \cdot \frac{2 D_{AB}}{\cancel{k_L}} \frac{\rho_T}{\cancel{\rho_W}} \frac{1}{\delta_m} = \frac{1}{w_{AS}} \frac{d}{dt}\left[\rho_T w_{AS} \frac{\delta_m}{3}\right]$$

$$6 D_{AB}\left(\frac{1}{\delta_m}\right) = \frac{d\delta_m}{dt} + \frac{\delta_m}{w_{AS}} \frac{d w_{AS}}{dt} \qquad (4)$$

But by differentiating eq. ③

$$\frac{d w_{AS}}{w_{AS}} = -\gamma\, d\left(\frac{1}{\delta_m}\right)\left[\frac{1}{1+\gamma/\delta_m}\right]$$

substitute into eq. ④

$$\frac{6 D_{AB}}{\delta_m} = \frac{d\delta_m}{dt} - \frac{\delta_m \gamma}{1+\gamma/\delta_m} \frac{d\left(\frac{1}{\delta_m}\right)}{dt}$$

$$6 D_{AB} = \delta_m \frac{d\delta_m}{dt} + \frac{\cancel{\delta_m}\gamma}{1+\gamma/\delta_m} \frac{1}{\cancel{\delta_m}} \frac{d\delta_m}{dt}$$

$$= \delta_m \frac{d\delta_m}{dt} + \frac{\delta_m \gamma}{\delta_m + \gamma} \frac{d\delta_m}{dt}$$

Integrate subject to $\rightarrow$ at $t=0$, $\delta_m = 0$

$$6 D_{AB} t = \frac{1}{2}\delta_m^2 + \int_0^{\delta_m} \frac{\delta_m \gamma}{\delta_m + \gamma}\, d\delta_m$$

$$6 D_{AB} t = \frac{\delta_m^2}{2} + \gamma \delta_m - \gamma^2 \ln\left(\frac{\delta_m + \gamma}{\gamma}\right) \; ; \; \gamma = \frac{2 D_{AB} \rho_T}{k_L \, \rho_w}$$

Above is $\delta_m(t)$. Also $w_{AS} = w_{A\alpha}\left(\delta_m / (\delta_m + \gamma)\right)$

Subst. into $w_A / w_{AS} = (1 - x/\delta_m)^2$ for profile ⟶

b After time t, the total amount DMSO absorbed:

$$\frac{Q}{m^2} = \int_0^{\infty} \rho_T w_A \, dx$$

$$= \rho_T w_{AS} \int_0^{\delta_m} \left(1 - \frac{x}{\delta_m}\right)^2 dx$$

$$= \rho_T w_{AS} \delta_m \int_0^1 (1-\eta)^2 d\eta \quad ; \quad \eta = x/\delta_m$$

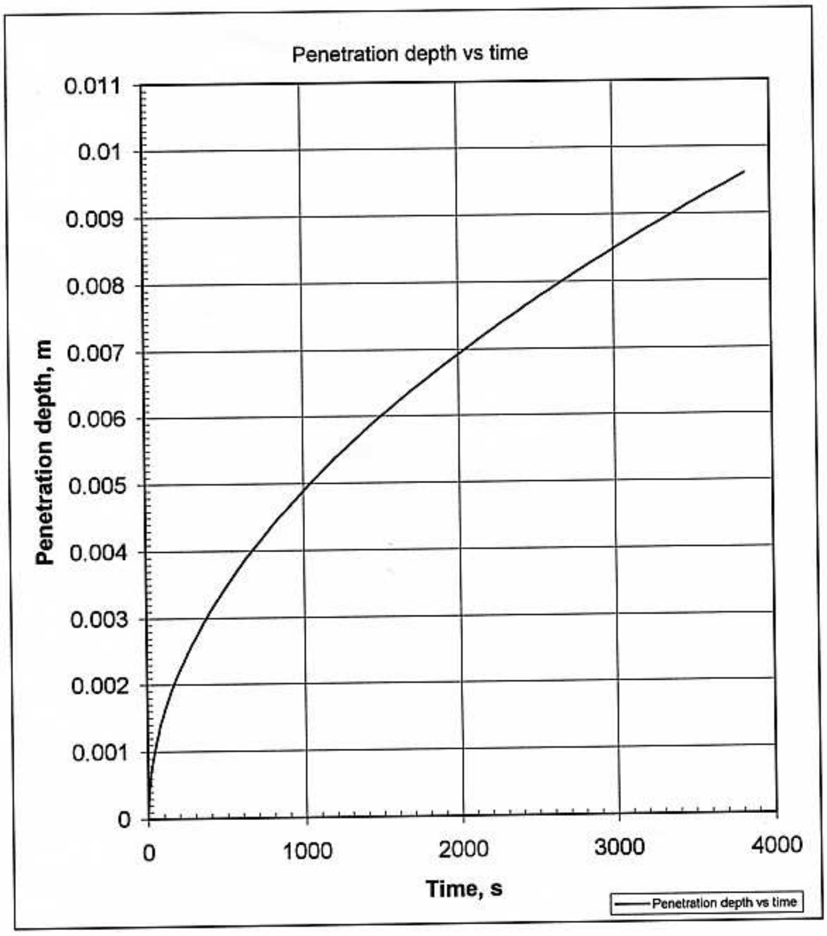
$$= \rho_T w_{AS} \delta_m / 3$$ ⟶

$\gamma = 3.4215(10^{-6})$

δ_m, m	t, s	$w_{AS} = w_{A\alpha}\left(\frac{\delta_m}{\gamma + \delta_m}\right)$
0	0	0
0.001	41.95	0.019932
0.002	167.23	66
0.003	375.85	77
0.004	667.8	83
0.005	1043.1	86
0.006	1501.7	89
0.007	2043.66	99

$t = 1800$ s or 30 min, $\delta_m \simeq 0.00656$ m, $w_{AS} = 0.01999$

$$Q/m^2 = \frac{1035 \cdot (0.01999)(0.00656)}{3} = 0.0452 \text{ kg/m}^2 \text{ area}$$ ⟶


Penetration depth vs time
0.011
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
Penetration depth, m
0
1000
2000
3000
4000
Time, s
Penetration depth vs time

List One

t	δ	w_{AS}
Time, s	P. D., m	Mf-surf
0	0	0
0.441854	0.0001	0.019338
1.719706	0.0002	0.019664
3.831162	0.0003	0.019774
6.776063	0.0004	0.01983
10.55436	0.0005	0.019864
15.16603	0.0006	0.019887
20.61106	0.0007	0.019903
26.88944	0.0008	0.019915
34.00117	0.0009	0.019924
41.94625	0.001	0.019932
50.72467	0.0011	0.019938
60.33643	0.0012	0.019943
70.78153	0.0013	0.019947
82.05997	0.0014	0.019951
94.17175	0.0015	0.019954
107.1169	0.0016	0.019957
120.8953	0.0017	0.01996
135.5071	0.0018	0.019962
150.9522	0.0019	0.019964
167.2307	0.002	0.019966
184.3425	0.0021	0.019967
202.2876	0.0022	0.019969
221.0661	0.0023	0.01997
240.6779	0.0024	0.019972
261.123	0.0025	0.019973
282.4015	0.0026	0.019974
304.5133	0.0027	0.019975
327.4585	0.0028	0.019976
351.237	0.0029	0.019976
375.8488	0.003	0.019977
401.2939	0.0031	0.019978
427.5724	0.0032	0.019979
454.6842	0.0033	0.019979
482.6294	0.0034	0.01998
511.4078	0.0035	0.01998
541.0197	0.0036	0.019981
571.4648	0.0037	0.019982
602.7433	0.0038	0.019982
634.8551	0.0039	0.019982
667.8003	0.004	0.019983
701.5788	0.0041	0.019983
736.1906	0.0042	0.019984
771.6357	0.0043	0.019984
807.9142	0.0044	0.019984
845.0261	0.0045	0.019985
882.9712	0.0046	0.019985

List Two

921.7497	0.0047	0.019985
961.3615	0.0048	0.019986
1001.807	0.0049	0.019986
1043.085	0.005	0.019986
1085.197	0.0051	0.019987
1128.142	0.0052	0.019987
1171.921	0.0053	0.019987
1216.532	0.0054	0.019987
1261.978	0.0055	0.019988
1308.256	0.0056	0.019988
1355.368	0.0057	0.019988
1403.313	0.0058	0.019988
1452.092	0.0059	0.019988
1501.703	0.006	0.019989
1552.149	0.0061	0.019989
1603.427	0.0062	0.019989
1655.539	0.0063	0.019989
1708.484	0.0064	0.019989
1762.263	0.0065	0.019989
1816.874	0.0066	0.01999
1872.32	0.0067	0.01999
1928.598	0.0068	0.01999
1985.71	0.0069	0.01999
2043.655	0.007	0.01999
2102.434	0.0071	0.01999
2162.045	0.0072	0.019991
2222.491	0.0073	0.019991
2283.769	0.0074	0.019991
2345.881	0.0075	0.019991
2408.826	0.0076	0.019991
2472.605	0.0077	0.019991
2537.216	0.0078	0.019991
2602.662	0.0079	0.019991
2668.94	0.008	0.019991
2736.052	0.0081	0.019992
2803.997	0.0082	0.019992
2872.776	0.0083	0.019992
2942.387	0.0084	0.019992
3012.833	0.0085	0.019992
3084.111	0.0086	0.019992
3156.223	0.0087	0.019992
3229.168	0.0088	0.019992
3302.947	0.0089	0.019992
3377.558	0.009	0.019992
3453.004	0.0091	0.019992
3529.282	0.0092	0.019993
3606.394	0.0093	0.019993
3684.339	0.0094	0.019993
3763.118	0.0095	0.019993
3842.729	0.0096	0.019993