

ME6203 MASS TRANSPORT

Examples of Math Modeling- Two Biomed Applications

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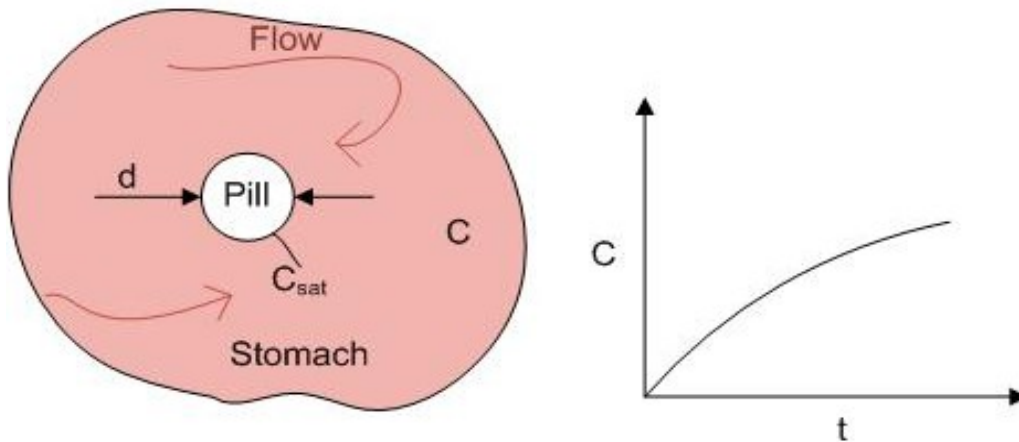
Math modeling of simple mass transfer problems – Illustrations

1) Estimate the average flow rate (velocity) in the stomach by measuring dissolution rate of a non-absorbing solute in the form of a spherical pill. Analyze the problem and explain how this could be done. State the assumptions. Assume net flow out of the stomach is negligible. (Sometimes referred to a churn flow)

Solution:

Assumptions

- 1) Dissolution rate expressed adequately by a mass transfer coefficient. “ k ”.
- 2) Pill remains spherical, same diameter over length of the experiment.
- 3) Stomach contents can be sampled with time
- 4) No chemical reaction



- 5) Mass flux is proportional to concentration driving force

As time increases, C of solute in the stomach increases.

Abbreviated solution.

- 1) Rate of dissolution $\sim k(c_{sat} - c) \cdot \pi d^2$, c_{sat} is the solubility of solute in stomach fluids at body temperature; c is the concentration of solute at time t .
- 2) Rate of accumulation of solute in stomach fluid $= V \frac{dc}{dt}$ where V is the volume of stomach fluids which is **constant**.

Equating the terms in (1) and (2) and integration by subjecting the equation to the initial

condition $C=0$ at $t=0$, gives, $k = \frac{V}{\pi d^2 t} \ln \frac{c_{sat}}{(c_{sat} - c)}$

If we can estimate k then we can estimate t !

Now, k can be obtained from a suitable empirical correlation for mass transfer from a sphere.

Sherwood number, $Sh = \frac{kd}{D} = 2 + 0.6 \left(\frac{dv}{\nu} \right)^{1/2} \left(\frac{\nu}{D} \right)^{1/3}$, where

$\left(\frac{dv}{\nu} \right) = Re$, Reynolds number and

$\left(\frac{\nu}{D} \right) = Sc$, Schmidt number

Hence the unknown velocity “ ν ” of stomach fluids is the given by

$$\nu = \frac{25}{9} \left(\frac{\nu^{1/3} D^{2/3}}{d} \right) \left[\frac{V}{\pi d t D} \left(\frac{c_{sat}}{c_{sat} - c} \right) - 2 \right]$$

This is at best an estimate! Note solution is only as good as the assumptions!

Question:

Is it possible to use a diffusion model to solve the problem posed? Explain briefly your response.

2) Biomedical application –Illustration 2

Write a math model for dissolution of a pill (assume diffusion-controlled; stagnant surroundings) in the stomach fluids so as to estimate the rate at which the drug permeates the body. Estimate the time required to reduce the transient contribution to the dissolution rate to less than 10% of the steady state term (in the solution). Assume the solution is dilute and the drug is sparingly soluble in the surrounding fluids.

Abbreviated Solution:

Assumptions:

- 1) Mass transfer flux \propto Concentration gradient of solute
- 2) Uniform drug release (within 10%)
- 3) Diffusion within the pill is negligible.
- 4) Diffusion in the surroundings is negligible.
- 5) Pill is spherical and remains so without change of diameter.

One dimensional diffusion equation in spherical coordinates is given by: (justify!)

$$\frac{\partial c_1}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_1}{\partial r} \right)$$

subject to the following IC and BC's

1) IC $t=0, r=r, c_1=0$

2) BC $t>0, r=R_0; c_1=c_1(sat)$

$r \rightarrow \infty; c_1=0$ (Assumes drug is quickly removed by interstitial wall;
rate limiting step is dissolution rate. $\therefore k \rightarrow \infty$)

(For solution to the pde refer to any book on conduction/diffusion e.g. by Crank, Ozisik etc.). If we define a new variable u such that

$u = \frac{c_1}{r}$; converts to cartesian problem

Soln:
$$\frac{c_1}{c_1(sat)} = \frac{R_0}{r} \left(1 - \operatorname{erf} \frac{r - R_0}{\sqrt{4Dt}} \right)$$

Note: $\operatorname{erf}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-\eta^2} d\eta$; $\operatorname{erf}(\infty) = 1$; $\operatorname{erf}(-x) = -\operatorname{erf}(x)$

Dissolution rate = $-D \frac{\partial c_1}{\partial r} \Big|_{r=R_0}$, **flux at surface**

$$= \frac{Dc_1(sat)}{R_0} \left(1 - \frac{R_0}{\sqrt{\pi Dt}} \right),$$

where the second term within the bracket represents the transient term.

For a nearly steady drug release rate,

$$\frac{R_0}{\sqrt{\pi Dt}} \ll 1$$

If we put $\frac{R_0}{\sqrt{\pi Dt}} = 0.10$, then

$$t_0 = \left(\frac{10R_0}{\sqrt{\pi D}} \right)^2$$

For $t > t_0$, transient contribution will be less than 10%.

If $D = 10^{-15} \text{ cm}^2/\text{s}$, $R_0 = 3 \text{ mm}$; $t_0 \sim 8 \text{ hours}$

But the actual value is $\sim 10 \text{ min}$. Hence this means that mass transfer is much more intensive and diffusion control is not a realistic mechanism.

Hence **BAD ASSUMPTIONS YIELD WRONG RESULTS**