**ABE 30800 Heat and Mass Transfer – Spring 2018**

**Homework 5 – TOTAL 140 marks**

**Due Thursday April 12**

**Problem 1**.

Consider a material that is wrapped to keep it from drying out. The moisture in the small amount of air inside the package will be at equilibrium with the moisture in the material. The system is 30oC and follows the equilibrium moisture curve whose data is given in the following table.

1. Plot moisture content of the material as a function of RH/100 (also known as water activity). What model can describe that moisture isotherm (use concepts provided in ABE 30300). Once the model is defined estimate their parameters (e.g. by Excel). You will need to determine the parameters of the moisture isotherm to determine the relative humidity inside the package (or water activity) in equilibrium with the moisture in the material. Since the moisture isotherm if far from be linear (illustrated in your plot) the use of linear interpolation to estimate the equilibrium RH may result in gross errors so you will need to find out the equilibrium RH as you learnt in ABE 30300 (e.g.by using Goalseek in Excel or the function root in Mathcad. Matlab also has several routines to estimate equilibrium RH.
2. The moisture in the material is 0.05 kg water per kg of dry solids. The outside air can be considered dried, i.e. has moisture zero (idealistic condition that will give an upper limit to the drying rate). Also assume air is blowing such that outside surface of the package is maintained at zero moisture. Calculate the loss of water vapor in grams/day at steady state for a wrapping of 0.1 mm thickness and a total surface area of 15cmx15cm. Assume that the diffusivity of water vapor in the packaging material is 0.4x10-11 m2/s and the density of the dry air is 1.1 kg/m3. Clearly specify your assumptions in solving this problem.

|  |  |
| --- | --- |
| **Relative Humidity of the Air**  **RH/100 = water activity** | **Moisture Content**  **(kg of water/kg dry solids)** |
| 0.008 | 0.026 |
| 0.014 | 0.040 |
| 0.028 | 0.060 |
| 0.043 | 0.075 |
| 0.056 | 0.10 |
| 0.070 | 0.12 |

**[40 marks]**

**Problem 2.**

Steady state diffusion of a component through a solid matrix with a spherical geometry can be calculated using the concept of resistance to the mass transfer. The approach is similar than what you have done on energy transfer where the variable was the temperatures, now it is replaced by the concentration of the diffusing component. You will need to find the equation that allows you to estimate the mass (or moles) flow in kg/s (or moles/s) using the Equation , in other words you will need to find out what is the expression of the resistance to estimate the molar flow NA. for that you can follow the following steps;

1. Start with the general microscopic mass balance equation to estimate the mass transfer of the species A. By making suitable assumptions you can find a differential equation to get the concentration profile of the species A in the spherical tablet. In addition to the differential equation you will need concentration specified boundary conditions at the inner, *Ri*, and outer, *Ro*, radii which are written as:

* *c(r=Ri) = Ci*at *r = Ri*
* *c(r=Ro) = Co at r =Ro*

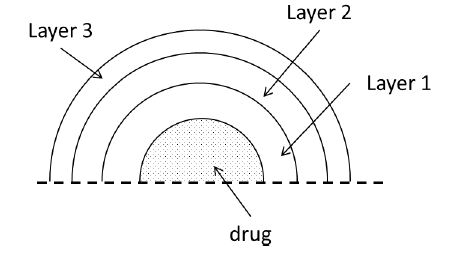
1. With the concentration profile (*cA* as a function of *r*) or the species A, obtain an equation to calculate the flow of A (by diffusion) through the layer.

(3) Rewrite the expression of the flow of A in terms of a concentration difference divided by a resistance and thereby obtain the expression for the resistance.

(4) Now you need to extend the problem to a multilayer tablet. The schematic of a drug spherical tablet is shown in the figure below. The main ingredient of the drug is Naxoproxen Sodium (the component/species A for this problem) that diffuses through various layers of a spherical drug tablet, which among other things are designed to provide a more uniform release of the active ingredient out of the tablet. The thickness of the layers 1, 2 and 3 and their diffusivities are shown in the table below:

|  |  |  |
| --- | --- | --- |
| **Layer** | **Thickness (mm)** | **Drug Diffusivity (mm2/s)** |
| 1 (Methocel K100) | 1.00 | 10 x 10-2 |
| 1 (Methocel E10) | 0.90 | 0.2x10-2 |
| 3 (PVA) | 0.15 | 0.35x10-2 |

Calculate the flow rate of A (in mg/s) from the outer surface when all three layers are considered in the drug transport, using the data in the table. The inner concentration of the layer 1 is 1 mg/mm3 and the outer surface concentration of layer the layer 3 can be considered zero. The radius of the drug is 5mm.



**[40 marks]**

**Problem 3.**

The section of human skin can be simply represented as a slab, known as the ***stratus corneum***. For the simplified case of medication transport through skin, assume the total diffusional resistance of the skin to the transfer of the drug is entirely due to the ***stratum corneum*** and none through other components of the skin, such as the sweat ducts, etc. Consider application of a medication to the surface of skin, maintaining a concentration of 15μg/cm3 of the medication at the skin surface. The inner surface of the ***stratum corneum*** is assumed to be maintained at essentially zero concentration since the molecules are removed as soon as they reach the microcirculation by a sufficiently high peripheral blood flow through skin in the human body.

(1) Calculate the flux of medication through the skin at steady state.

(2) Calculate how much of the medication resides in the ***stratum corneum*** per unit skin area at steady state. The thickness of the stratum corneum is 1. The diffusivity of the medication (a low-molecular weight non-electrolyte) through the ***stratum corneum*** is 10-10 cm2/s.

**[20 marks]**

**Problem 4.**

In addition to its function as a physical barrier, the skin also acts as a metabolic barrier capable of degrading a wide variety of compounds upon penetration by diffusion. Consider a drug diffusing through the skin where metabolic reactions cause the drug to be eliminated as a first order reaction with a constant k= 1000 1/min. The diffusivity of the substrate in the skin tissue is 2x10-10 m2/s. The substrate concentration at the surface is 300 nmol/ml. The thickness of the metabolizing skin tissue is thick enough such that the concentration reaches zero before full thickness.

1. Write the equations to estimate the drug diffusion and elimination along the boundary conditions
2. Write the solution of the equation, i.e. concentration as a function of position and substitute in the equation the appropriate numerical values.
3. Find the depth of penetration, defined as the distance at which concentration of the drug is 10% of its surface value
4. Find the rate of **drug flux** in nmol/m2.s at which the drug penetrates the skin surface
5. What is the depth of penetration when the drug is consumed at twice the rate given by *k*, i.e. when the first order constant changes to 2*k*?
6. When the consumption of the drug double to 2*k* (as in 5) and you still want to have the same concentration at the same depth as in question (3), what two parameters would you change, how and by how much?

**[40 marks]**