CHEN 6603 Homework 13

<u>Mass Transfer with Reaction in Pores</u>: Ethylene Oxide Synthesis

For the following problem, produce a memo report including your iPython code to solve the problem.

Ethylene Oxide is a toxic gas that leaves no residue on items it contacts. It is a surface disinfectant that is widely used in hospitals and the medical equipment industry to replace steam in the sterilization of heat-sensitive tools and equipment, such as disposable plastic syringes. Sterilization by ethylene oxide for the preservation of spices was patented in 1938 by the American chemist Lloyd Hall. Ethylene oxide achieved industrial importance during World War I as a precursor to both the coolant ethylene glycol and the chemical weapon mustard gas. It is so flammable and extremely explosive that it is used as a main component of thermobaric weapons.

Direct oxidation of ethylene by air was invented and patented by the French scientist Lefort in 1931 and in 1937 Union Carbide opened the first plant using this process. It was further improved in 1958 by Shell Oil Co. by replacing air with oxygen and using elevated temperature of 200–300 °C (390–570 °F) and pressure (1–3 MPa (150–440 psi)). This more efficient routine accounted for about half of ethylene oxide production in the 1950s in the US, and after 1975 it completely replaced the previous methods. But even when oxygen is used, nitrogen is often added to control the reactor temperature due to the exothermic oxidation reactions. The production of ethylene oxide accounts for approximately 11% of worldwide ethylene demand.

The Lefort Process combines nitrogen (component 1) and oxygen (component 2), with ethylene (component 3) to form ethylene oxide (component 4), carbon dioxide (component 5) and water vapor (component 6) over a silver-based catalyst through the following two reactions:

$$2C_2H_4 + O_2 \dashrightarrow 2C_2H_4O \quad \text{(Equation 1)}$$
$$C_2H_4 + 3O_2 \dashrightarrow 2CO_2 + 2H_2O \quad \text{(Equation 2)}$$

The catalyst for the reaction is metallic silver deposited on various matrixes, including pumice, silica gel, various silicates and aluminosilicates, alumina and silicon carbide, and activated by certain additives including antimony, bismuth, barium peroxide, etc. These cylindrical catalyst of 5mm average diameter are shown in the image above.

The average pore size of the catalyst has been measured and is represented by pores of 4 microns in diameter and have a characteristic length of 1mm.

The reaction rate of C_2H_4 from reactions 1 and 2 above proceeds as:
$r_1 = k_1 c_1 c_2^2 / F_1^2$ where k_1= 8.63 x 10^7 mol/s cm^3
$r_2 = k_2 c_1 c_2^2 / F_2^2$ where k_2= 6.57 x 10^7 mol/s cm^3
and where c_1 is the concentration of C_2H_4 and c_2 that of O_2, both in mols/cm^3.
$F_1 = (0.0106 + 2144c_1 + 805c_2)(1 + 1271\sqrt{c_2})$
$F_2 = (0.008 + 4166c_1 + 1578c_2)(1 + 718\sqrt{c_2})$

Consider a packed bed tubular reactor sized as follows:
- Tube diameter = 0.03912 m
- Tube length = 12.8 m
- Number of tubes = 2781
- Total available catalyst surface area = 4396 m^2
- Total reactor volume = 43 m^3
- Catalyst density = 881 kg/m^3
- Catalyst per reactor = 9431 kg

The molar flow to the reactor (kmol/hr) is:
- Ethylene = 80.5
- Nitrogen = 1274
- Carbon dioxide/Ethylene oxide/Water = 0
- Oxygen = 91.5

The heat transfer correlation based on this diameter for these catalyst cylinders has been obtained as:

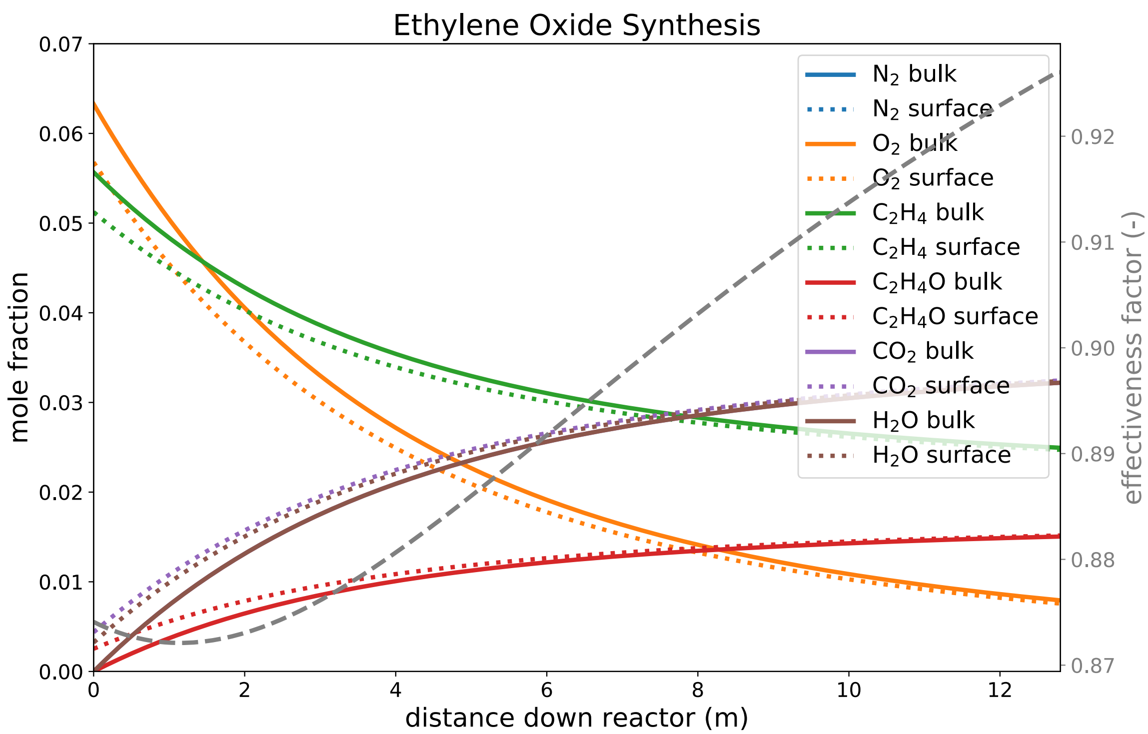
$$\overline{Nu}_D = c\,\mathrm{Re}_D^m\,\mathrm{Pr}^{1/3} \qquad \text{(Equation 3)}$$

Table 9.1 Constants of Equation 3 at different Reynolds numbers

Re_D	c	m
0.4-4	0.989	0.33
4-40	0.911	0.385
40-4000	0.683	0.466
4000-40,000	0.193	0.618
40,000-400,000	0.027	0.805

The synthesis is performed at a pressure of 2 atm and at a temperature of 228 Celsius. The gas mixture dynamic viscosity at these conditions is 4x10-5 m^2/s.

What is the mole fraction profile through the reactor?
What is the effectiveness factor profile through the reactor?
What is the fractional yield of desired product (ethylene oxide) from the ethylene as a function of distance through the reactor?



As can be seen from the plot below, these pores are large enough to allow all the surface area to be available without any Knudsen diffusion effects. The pores need to be one order of magnitude smaller to cause Knudsen diffusion effects (try it in your code).