

- 1a. X = conversion
 W = catalyst weight

Balance equation for a packed bed reactor:

$$\frac{dX}{dW} F_{Cl_2} = -r_{COCl_2}$$

from the problem statement we have:

$$-r_{COCl_2} = k P_{CO} \frac{P_{Cl_2}}{AP_{CO} - P_{COCl_2}} \quad \forall$$

Substituting in we have:

$$\frac{dX}{dW} F_{Cl_2} = k P_{CO} \frac{P_{Cl_2}}{AP_{CO} - P_{COCl_2}} \quad \forall$$

Converting from partial pressures: at any point along the reactor we know that-

$$y_{CO} = \frac{N_{CO}^o - XN_{Cl_2}^o}{N_{CO}^o + N_{Cl_2}^o - XN_{Cl_2}^o}$$

$$P_{CO} = y_{CO} P$$

$$y_{Cl_2} = \frac{N_{Cl_2}^o - XN_{Cl_2}^o}{N_{CO}^o + N_{Cl_2}^o - XN_{Cl_2}^o}$$

$$P_{COCl_2} = y_{COCl_2} P$$

$$P_{CO_2} = y_{CO_2} P$$

$$y_{COCl_2} = \frac{XN_{Cl_2}^o}{N_{CO}^o + N_{Cl_2}^o - XN_{Cl_2}^o}$$

Extent of reaction: $XN_{Cl_2}^o$

$$N_T = N_{CO}^o + N_{Cl_2}^o - XN_{Cl_2}^o$$

$$N_{CO} = N_{CO}^o - XN_{Cl_2}^o$$

$$N_{Cl_2} = N_{Cl_2}^o - XN_{Cl_2}^o$$

$$N_{COCl_2} = XN_{Cl_2}^o$$

Divide through by $N_{Cl_2}^o$ and let $Y = N_{CO}^o / N_{Cl_2}^o$

$$y_{COCl_2} = \frac{X}{Y + 1 - X} \quad y_{Cl_2} = \frac{1 - X}{Y + 1 - X} \quad y_{CO} = \frac{Y - X}{Y + 1 - X}$$

$$\frac{dX}{dW} F_{Cl_2} = k \frac{P}{F_{Cl_2}^o} \frac{Y - X}{Y + 1 - X} \frac{1 - X}{A(Y - X) + X} \quad \frac{1}{4}$$

From the problem statement we know that $Y=2$
We also know that the pressure drop is linear.

$$P = P_{out} - \frac{P_{out} - P_{in}}{W_{total}} W$$

Calculating the constants and doing the conversions:

$$P_{out} = 1 \text{ atm}$$

$$P_{in} = 1.3 \text{ atm}$$

$$k = k_o \exp(-E / RT) = 22.6 \frac{\text{mol}}{\text{h m}^2 \text{ atm}} \times \frac{850 \text{m}^2}{\text{g}} \times \exp\left(-\frac{7570 \text{cal}}{1.987 \text{cal/mol/K} \cdot 448 \text{K}}\right)$$

$$k_{448\text{K}} = 3.89 \text{ mol/h/g/K}$$

$$A = 10^{\left(\frac{-1900}{T} + 3.4\right)}$$

$$A_{448\text{K}} = 0.144$$

$$F_{Cl_2}^o = 4.5 \text{ sccm} / 3 = 1.5 \text{ sccm}$$

convert to moles per time using standard conditions of 1atm, 273 K

$$PV = nRT \rightarrow$$

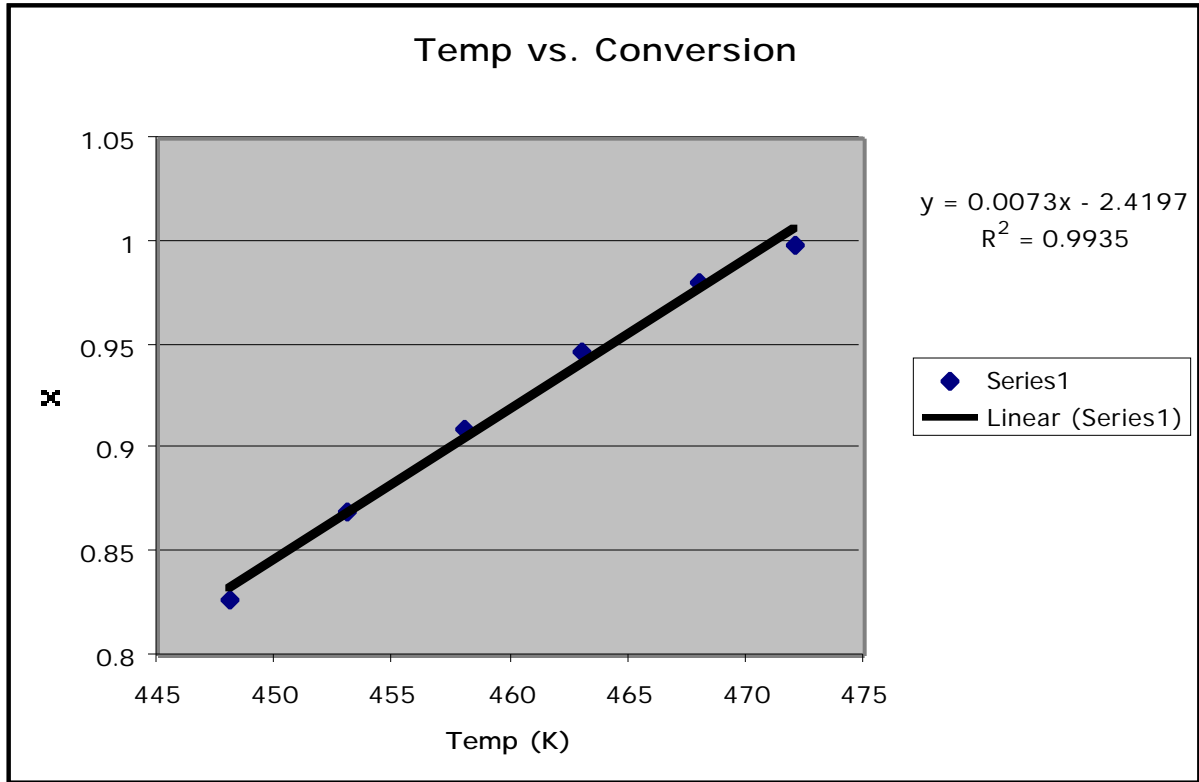
$$n = \frac{1 \text{atm} \cdot 4.5 \text{cm}^3 / \text{min} \cdot 60 \text{min/hr}}{82.06 \text{cm}^3 \text{atm} / \text{mol} / \text{K} \cdot 273 \text{K}} = 0.004 \text{mol/hr}$$

Put these constants and the differential equation into Maple and use dsolve, type=numeric to solve the equation numerically. Then use plot(function) to plot X as a function of W. Use f(0.0013) to get a specific value for X at W=0.0013g. We see that at 175 degrees C, X=0.827. We also see that this is very close to the predicted value of 0.83.

(5 points for the derivation, 2 points for solving and plotting XvsW, 1 point for all the correct conversions, 2 points for the pressure drop equation, -1 point for correct approach but wrong answer)

1b. We can easily change T in the above equations, calculate new constants, and ask Maple to solve the equation again. If we plug in T=175, 180, 185, 190, 195, and 199 degrees C, we get conversions of 0.827, 0.869, 0.909, 0.947, 0.980, 0.9989 respectively. If we try 200 degrees, Maple should give an error message indicating that X>1 and we have a negative number to a fractional power. If we do iterations around 195-200, we see

that $X=0.995$ when $T=198$. If we plot the points using excel, we get a slightly different answer from the curve fit ($T=195$ degrees).



(3 points for showing the work and 2 points for the right number)

1c. First lets calculate how many channels would be required to give the desired output.

input=0.004 mol/hr

(input) \times (conversion) \times (1h/60min) \times (molecular weight of COCl₂)= grams of COCl₂ produced per reactor channel

output=0.0066 g/min

desired output/output per channel = number of channels required = 303 channels of the same size would be required to generate 2g/min of phosgene.

What happens if you change the reactor length? The pressure drop will change. For a longer channel, you need a greater inlet pressure. For a shorter channel, the pressure drop will be smaller. You could use catalyst posts instead of a packed bed to reduce the pressure drop. From looking at the graph of conversion versus reactor length/catalyst weight, the length seems to be in the appropriate range. The conversion does not level out halfway down the reactor nor is the end of the reactor reached while the slope of the conversion is still steep.

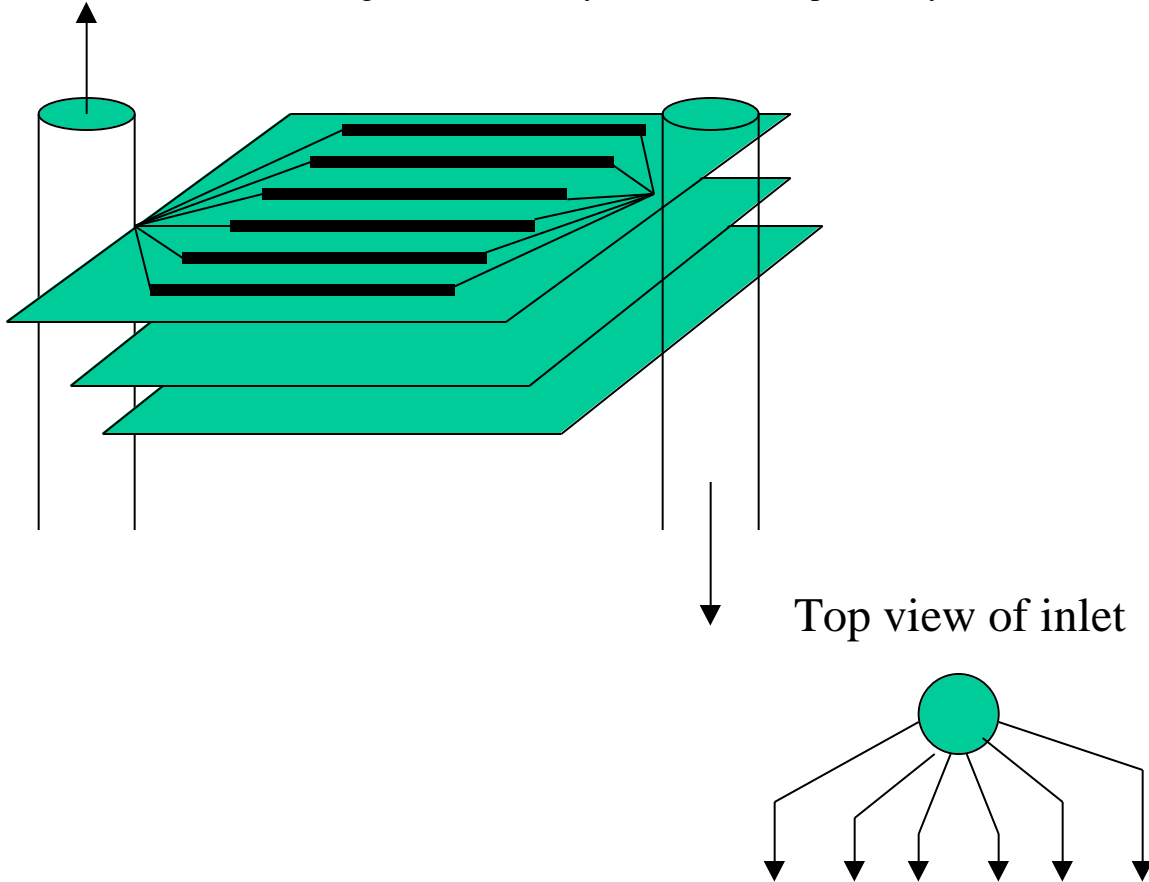
You can calculate the heat generation based on the given enthalpy of reaction.

$$H \times n = Q$$

$$26 \text{ kcal/mol} \times 0.004 \text{ mol/h} \times 1 \text{ h} / 60 \text{ min} = 1.7 \text{ cal/min}$$

This is actually quite small so even though the reaction is exothermic, the heat generation will be small and can possibly be used to heat the inlet streams .

Answers to the other design issues will vary, but here is one possibility:



Multiple channels can be microfabricated onto the same wafer and stacked along a larger manifold which provides the reactant streams. The width of the inlet channels must vary to maintain a constant inlet pressure to each reaction channel.

(3 points for calculating the number of channels, 3 points for discussing how all those channels can be fit together and how they should be connected to the inlet and outlet streams, 2 points for cooling calculation, 1 point for discussion of length, and 1 point for discussion of fabrication)