Pressure drop considerations are significant in the design of fixed-bed reactors. Exit pressures are often constrained by required conditions in downstream separations operations, and increases in inlet pressure often come at a cost (considering the cost of compression or pumping). A design guideline used for pressure drop in the specification of fixed-bed reactors is that the pressure drop should never exceed 1/10 of the initial pressure ($\Delta P \leqslant 0.1\ P_0$). Because pressure drop tends to increase in a bed over the life of the catalyst due to particle attrition and breakage, this guideline should be used as an absolute upper limit to design for pressure drop.

The reactor of choice for these partial oxidation reactions we are focusing on in this project is the multi-tubular fixed-bed reactor. For highly exothermic reactions, multi-tubular reactors offer the advantage of good heat transfer due to the small diameter of individual tubes, and the opportunity to optimize pressure drop by manipulating the number of tubes needed to achieve your target reactor volume. Remember that this reactor will need to be fabricated, transported and installed, so practical a reactor length should be considered.

For Memo 2 you developed a simple model for an isothermal reactor using a single reaction and a single mole balance equation using POLYMATH, and you developed a simple plug flow model using Aspen Plus®. In this memo, you will expand your POLYMATH model to include the momentum balance (pressure drop equation) using the Ergun equation (see Fogler) and then explore the relationship between pressure drop and number of tubes.

1.   Present a preliminary design of your reactor based on the kinetics used in Memo 2 (and given again below). Use POLYMATH for this portion of the reactor design. Your model **must** contain at least **one mole balance** and a **momentum balance** (pressure drop) using the Ergun equation.

   1.1.   Assume that you have an isothermal reactor with the approximate reactor volume determined in Memo 2.[1] Create the plots of conversion vs. volume (or catalyst weight) for contours of constant temperatures for your selected temperature range, as done in Memo 2. Select a catalyst particle size and bed void fraction based on your literature search, and document this reference. (If you don't have values for these, 5mm particles with 0.4 void fraction is a good place to start[2]).
   Comment on the differences when pressure drop is a consideration.

   1.2.   Now using your target reactor 'conversion' and resultant catalyst weight (reactor volume), explore the relationship between the number of tubes and pressure drop. Select a reasonable reactor length (use 3—3.5 meter length) and 1" tubes. Select a catalyst particle size based on your literature search, and document this reference. (If you use too few tubes, you'll have convergence problems).
      1.2.1.   Determine number of tubes necessary to obtain your target reactor volume and calculate pressure drop. Explore reactor length vs. pressure drop for a fixed reactor volume, so for each reactor length, your tube number will change at constant total volume. ***Plot ΔP vs. L for a given catalyst particle size.***
      1.2.2.   For comparison, increase your particle size by a factor of two and create the same ΔP vs. L plot.
   1.3.   Provide sample calculations of your numerical model (*e.g.,* conversion factors, differential equations and boundary conditions. For example give sample calculations equation given in your Polymath code.
   1.4.   Include references for all data (conversion used, inlet T and P, approximate reactor volume etc.).
   1.5.   ***Include a discussion of these runs and results.***

Reaction Kinetics
   Use the kinetics assumed in memo 2 for this work.

   a)   **Reaction kinetics for the air oxidation of benzene to maleic anhydride:**

   Assume the rate law is half-order in benzene for the following stoichiometry and rate parameters:

$$C_6H_6\ +\ 4\ O_2\ \xrightarrow{\ k_1\ }\ C_4H_2O_3 + 2\ H_2O + CO_2 + CO$$

   The rate is: $r_M = k \cdot C_B^{1/2}$, where k is the rate constant for this simplified reaction model and C_B is the concentration of benzene ([kmol/m3] = [M]).

$$k = 8.20766 \cdot 10^7\ \exp(\text{-}19618/T)\ [\text{m}^3/\text{kgcat-M}^{-1/2} - \sec]$$

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[1] Since these are one-dimensional reactor models, the length to diameter ratio are insignificant to overall reaction conversion and selectivity – only overall volume or catalyst weight is important. The aspect ratio will impact pressure drop, however, and both Polymath and Aspen+ will have trouble converging numerically if the pressure drop is too large. So, starting with a shorter, fatter reactor will help you approach your optimum L/D because you'll be able to get results.

[2] Our target multi-tubular reactor for highly exothermic reactions will use 1" tubes. Often a 10:1 d_t/d_p ratio is adopted for optimal flow characteristics and particle wetting, however, because heat transfer is important with large the exotherms, a ratio of 4-5 has been shown to be optimal.

b) **Reaction kinetics for the air oxidation of butane to maleic anhydride:**

Assume the rate law is pseudo-first order in butane for the following stoichiometry and rate parameters.
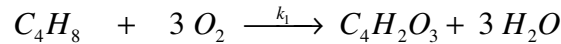
$$C_4H_{10} + 3.5\,O_2 \xrightarrow{\ k_1\ } C_4H_2O_3 + 4\,H_2O$$
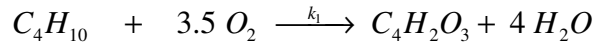
The rate is: $r_M = k_1 \cdot C_B$, where k_I is the pseudo-first order rate constant and C_B is the concentration of butane.

$$k_1 = 8.1048 \cdot 10^6 \ \exp(-15649/T) \ \ [m^3/kgcat\text{-}sec]$$

c) **Reaction kinetics for the air oxidation of butene to maleic anhydride:**

Assume the rate law is pseudo-first order in butene for the following stoichiometry and rate parameters.

$$C_4H_8 + 3\,O_2 \xrightarrow{\ k_1\ } C_4H_2O_3 + 3\,H_2O$$

The rate is: $r_M = k_1 \cdot p_B$, where k_1 is the pseudo-first order rate constant and p_B is the partial pressure of butene [bar].

$$k_1 = 3.8075 \cdot 10^5 \ \exp(-11569/T) \ \ [kmol/kgcat - bar - sec]$$

d) **Reaction kinetics for the air oxidation of propylene to acrolein:**

Assume the rate law is first order in propylene and half order in O_2, for the following stoichiometry and rate parameters.

$$C_3H_6 + O_2 \xrightarrow{\ k_1\ } C_3H_4O + H_2O$$
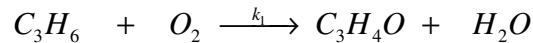
The rate is: $r_A = k \cdot C_P \cdot C_{O_2}^{1/2}$, where k is the rate constant and C_P and C_{O_2} are the concentrations of propylene and O_2, respectively.

$$k_1 = 5.1778 \cdot 10^6 \ \exp(-16206.5/T) \ \left[m^3_{rxtr}/kgcat - sec - \left(kmol/m^3\right)^{1/2} \right]$$

If you choose, you can begin to use a reaction rate that you have found in the literature (with proper attribution) instead of the above rates, but contact Dr. LaMarca for approval of your selected kinetics.

2. Present a preliminary design of your reactor based on the kinetics used in part 1 using Aspen Plus® and the RPLUG reactor block incorporating the pressure drop Ergun correlation as done in your lab. Assume that you have an isothermal reactor with initial conditions identical to those used in your POLYMATH model above. For each run include a report file[3].
   2.1. Use the reactor volume determined in part 1 for your productivity rate and reaction chemistry.
      2.1.1. For your first run, assume a single reactor tube with configuration used in part 1.1.
      2.1.2. For your next run, assume a multi-tubular reactor with the configuration determined in part 1.2.
   2.2. *Compare these results with those developed in POLYMATH, and comment on differences. Include all assumptions for your modeling as well as the references for these assumptions in your summary as well.*
   2.3. *Generate a report file for each run and send both the report files and the *.bkp file electronically to Dr. LaMarca as an e-mail attachment.*
3. Present a preliminary evaluation of the reaction rates expressions that you have obtained from the literature for use in your reactor for **approval by Dr. LaMarca**. This will consist of hand calculations of the reaction rates at your reactors initial conditions. You must compare your hand calculations with results given in the paper. Your reaction rates should have the ability to predict byproducts of your reaction. These reaction rates must be obtained from a journal source. Many of the journal articles that you will need for this project can be obtained from the Library, Interlibrary Loan or ScienceDirect (Elsevier). Remember, you may use as a starting point: *Rate equations of solid-catalyzed reactions*, edited by Reiji Mezaki and Hakuai Inoue. Tokyo, University of Tokyo Press, c1991. Call#: QD502.R38 1991. *You will need to use these rate expressions in Memo 4.*

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[3] Once the simulation run is complete, select Export from the File menu (also Ctrl E). Under the 'Save as Type' field, select the Report Files (*.rep). This file will have the name of your simulation with a .rep extension. This will generate a report file that you should print.