**1)** Develop an *isothermal* reactor model to estimate the reactor volume for the production of maleic anhydride or acrolein by the partial air oxidation of your group's feedstock at your prescribed production rate. Develop a packed bed reactor model as a function of catalyst weight, and then convert the determined weight to a reactor volume using a suitable catalyst bulk density[1]. You should use typical inlet compositions of benzene, butane, butene or propylene and typical reaction selectivity to maleic anhydride or acrolein determined in your background work for the first memo. In this memo we will explore a reactor with a single reaction, however, reactions to byproducts will be added as we proceed through the semester.

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:

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

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]).

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

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.

$$C_4H_{10} \quad + \quad 3.5\ O_2 \xrightarrow{k_1} C_4H_2O_3 + 4\ H_2O$$

The rate is: $r_M = k_1 \cdot C_B$, where $k_1$ is the pseudo-first order rate constant and $C_B$ is the concentration of butane.

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

**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.

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

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].

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

**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.

$$C_3H_6 \quad + \quad O_2 \xrightarrow{k_1} C_3H_4O \ + \quad H_2O$$

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.

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

Submit the solution to this problem using Polymath and show the derivation of each equation used. (An electronic copy of your Polymath model should supplement your memo submission). Give hand calculations of each representative calculation. (*e.g.* should provide a sample calculation of the ODE's evaluated at the initial conditions).

[1] Your catalyst bulk density, which includes the voids upon packing in the reactor, should be in the neighborhood of 1000 kg-cat/m3-rxtr.

2) For your reaction system, explore the effect of temperature and reactor volume (catalyst weight) on conversion using your Polymath model. Create plots of conversion vs. volume (or catalyst weight) for contours of constant temperature over a temperature range of 350 – 450 °C.

3) Simulate your reactor using the Aspen Plus® ***RPLUG reactor*** block using the assumed reactor conversion used in part one of this exercise. These simulations will be introduced in next Thursday's laboratory, and more operational information will be provided during the lab period. Plot the effect of conversion of your reactant on the heat duty of an isothermal reactor.