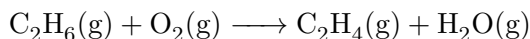


Carefully and neatly document your answers. You may use a mathematical solver like Jupyter/iPython. Use plotting software for all plots.

1 Too hot in here

Thermal ethane dehydrogenation, which you studied in the last homework, occurs at high T and is plagued by the generation of “coke,” or a cake of primarily carbon. An alternative way to create ethylene is through oxidative dehydrogenation:



At 600 K over some catalyst the reaction is half-order in ethane, first-order in O_2 , zero order in products, and has a pseudohomogeneous rate constant of $5.0 \text{ M}^{-1/2}\text{s}^{-1}$. (Note, I am completely making this up!) You plan to run the reaction in an isothermal, constant volume reactor starting with an 70:20:10 mixture of $\text{N}_2:\text{C}_2\text{H}_6:\text{O}_2$ at 2 bar total pressure.

1.1 Plot the rate of disappearance of C_2H_6 and of O_2 vs C_2H_6 conversion (don't forget to balance the reaction!).

1.2 Plot the concentrations of all species vs residence time in the reactor.

2 Not a laughing matter

Nitrous oxide (N_2O) decomposes to N_2 and O_2 at high temperature. Experiments were performed at constant T in a constant volume batch reactor. You can assume the reaction rate has the form $kP_{\text{N}_2\text{O}}^a$.

$P_{\text{N}_2\text{O},0}$ (torr)	T (K)	half-life (s)
82.5	1030	860
139	1030	470
296	1030	255
360	1030	212
345	1085	53
360	1030	212
294	967	1520

2.1 What is the reaction order?

2.2 What is the apparent activation energy?

3 I'm getting dehydrated

tert-butanol can be dehydrated to isobutylene over an ion-exchange resin. An experiment was performed to follow the concentration of butanol vs time at 338 K. You can assume the reaction rate is only dependent on the concentration of *tert*-butanol under these reaction conditions.

Time (h)	Butanol (M)
0	1.00
0.25	0.94
0.50	0.90
0.70	0.86
1.10	0.80
1.50	0.72
1.90	0.66
2.50	0.59
3.00	0.55
4.00	0.43
5.10	0.35
6.00	0.28

3.1 Write down the balanced reaction.

3.2 What is the reaction order?

3.3 What is the rate constant at this temperature?

4 Pressure packed

NH₃ synthesis from N₂ and H₂ was studied in a constant volume reactor (0.315 l) over a Ru catalyst, in a clever setup in which the NH₃ was continuously removed from the reactor. The total pressure in the reactor was followed vs time at three different compositions and at 350 °C. The pressures are reported as their equivalent values at 298 K (ie $N/V = P/R \times 298 \text{ K}$).

$$\text{N}_2:\text{H}_2:\text{He} = 3:1:0$$

Pressure (torr)	766.2	731.9	711.9	686.2	661.5
Time (min)	0	18	30	42	54

$$\text{N}_2:\text{H}_2:\text{He} = 1:1:2$$

Pressure (torr)	753.4	737.5	726.6	709.5	700.3
Time (min)	0	15	30	45	54

$$\text{N}_2:\text{H}_2:\text{He} = 1:3:0$$

Pressure (torr)	707.1	700.2	693.2	683.5	675.5
Time (min)	0	15	30	45	55

4.1 Write down the balanced reaction.

4.2 Plot the N₂ and H₂ concentrations (mol/vol) vs time for each initial condition.

4.3 Use finite differences to make a table of reaction rates (moles/time/volume) vs composition (mol/vol N₂ and H₂).

4.4 Use your rate data to determine a rate law and rate constant for the reaction at these conditions.