Homework 6
10.37 Spring 2007
Due Wednesday, March 21

Problem 1: Quoting from the Wilmington, DE *Morning News*, Aug. 3, 1977:

> "Investigators sift through the debris from blast in quest for the cause [why the new chemical plant exploded]. A company spokesman said it appears… likely that the [fatal] blast was caused by [rapid decomposition of] … ammonium nitrate [NH_4NO_3] used to produce nitrous oxide [N_2O]."

In the process, a $T=200^oF$ aqueous solution, 83 wt% ammonium nitrate, is fed into a CSTR. When the process is running normally at steady state, about 140 kg/hr of the aqueous solution is injected, and the temperature in the reactor, T_R, is 510^oF. At this temperature, the water evaporates rapidly, but the molten ammonium nitrate remains in the CSTR, slowly decomposing by this reaction:

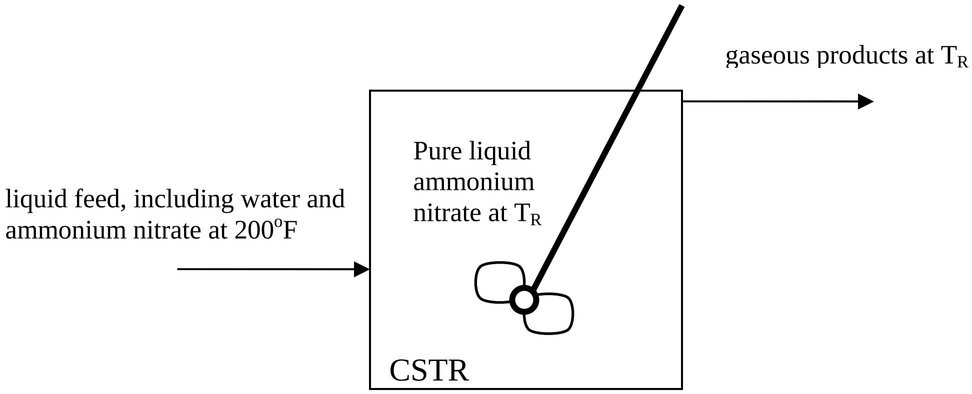
$$NH_4NO_3(\text{liquid}) \rightarrow N_2O(g) + 2\ H_2O(g)$$

$k(T=510^oF) = 0.307/\text{hour}$
$\Delta H_{rxn}(T=510^oF) = -740$ kJ/kg of ammonium nitrate

Note that it takes about 2.2 MJ to convert a kg of liquid water at 200^oF to a kg of steam at 500^oF.

Also, FYI:
Cp(steam) = 2 kJ/kg-degree F
Cp(liquid NH_4NO_3) = 0.8 kJ/kg-degree F

Neglect non-ideal mixing effects and assume that NH_4NO_3 enters as a liquid. Assume that ΔH_{rxn} is approximately constant in the reactor temperature ranges of the problem. A diagram is shown below.



(a) During normal steady-state operation, what mass (kg) of ammonium nitrate resides in the reactor? *Note that there is negligible hold-up of any gases within the reactor.*

(b) How much cooling capacity (in kW) is required for this reactor when it is running in steady state? If this is provided by excess cooling water with an average temperature T_a=100°F, what is the product of the heat transfer coefficient and the area, UA, in kW/F°?

During the investigation, it was hypothesized that the temperature increased, accelerating the reaction. The rate constant of the decomposition reaction increases with temperature, e.g. at T=560°F, k=2.91 hr^{-1}. The reaction follows the Arrhenius T-dependence.

(c) Using the stability criteria explained in the vicinity of Eq. 8-75, should the reactor operate stably at 510°F? What is the critical temperature above which runaway reaction could occur?

It is believed that pressure fluctuations were detected in the feed stream and it was shut off by a plant operator about 4 minutes before the explosion occurred.

(d) Write and (using Matlab) solve a set of differential equations describing what happened in the reactor after the feed was shut off. Plot the temperature in the reactor vs. time. Do you predict an explosion?

(e) Was the operator wise to quickly shut off the feed of aqueous ammonium nitrate solution when he feared something was going wrong in the reactor? Is there something else he should have done to prevent the disaster?

(f) Propose a procedure for safely starting-up and shutting-down a process like this (a qualitative description will suffice).