CE 561, Exam 2, December 22, 1998

The exam consists of two problems, each containing multiple parts. You will have two hours to work on it. The point value of each part of each problem is indicated at the end of the problem statement. Note these values, and budget your time accordingly. You may use a single sheet of notes (8.5×11 inches, both sides). A portion of a table of integrals and a table of values of the exponential integral are attached to the exam for your use as well.

Good Luck!

(1) Consider the production of SO_3 from SO_2 in a fixed bed tubular reactor. The overall reaction is $SO_2 + ½ O_2 \leftrightarrow SO_3$. The feed to the reactor is 3.0% by volume SO_2 and 97.0% by volume dry air (79% N_2, 21% O_2) at 400°C and 1.05 bar total pressure. The total feed flow rate is 2500 kg/hr. The reactor will be a 50 cm diameter cylindrical vessel filled with catalyst pellets. The platinum on alumina catalyst is in the form of 4 mm diameter cylindrical pellets (ranging from 15 to 50 mm long), with a catalyst density of 1.0 g cm^{-3}, a pore volume of 0.4 cm^3 g^{-1}, and a specific surface area of 150 m^2 g^{-1}. The density of the catalyst bed, as packed in the reactor, is 0.6 (kg catalyst) m^{-3}. The pressure drop through the reactor is negligible. The reaction rate, in the absence of any diffusion limitations, is

$r = k_1 C_{SO_2} - k_2 C_{SO_3}$, with

$k_1 = 1.0\times10^6 e^{(-12000/T)}$ m^3 s^{-1} (kg catalyst)$^{-1}$ and $k_2 = 1.0\times10^{13} e^{(-24000/T)}$ m^3 s^{-1} (kg catalyst)$^{-1}$. The specific heat of the gas mixture can be assumed constant at 1.0 kJ kg^{-1} K^{-1}. The atomic weights of sulfur, oxygen, and nitrogen are 32, 16, and 14 g mol^{-1}, respectively.

(a) Write the steady-state reactant (SO_2) mole balance equation and the enthalpy balance equation, including appropriate boundary conditions, for the fixed bed reactor for each of the following cases. Identify the variables in the equations and the units in which they are measured. Give their numerical values where possible. Where numerical values are not available from the problem statement, suggest how they might be obtained. For each part, give a **brief** description of how the balance equations could be solved numerically.

(i) Ideal plug flow, no radial or axial mixing, no heat flow through the reactor walls. (10 points)

(ii) Plug flow with mixing in the axial direction due to flow around the catalyst pellets, but still no heat flow through the reactor walls. (5 points)

(iii) Plug flow with both radial and axial mixing due to flow around the catalyst pellets and heat transfer through the reactor wall to condensing steam at 200 °C. (5 points)

(b) For *adiabatic operation* of the reactor with ideal plug flow and no radial or axial mixing, derive a relationship between the reactor temperature and the SO_2 conversion. Estimate the maximum temperature that could be reached in the reactor. What are the concentrations of SO_2 and SO_3 when this maximum temperature is reached? (10 points)

(c) Calculate the Thiele modulus and estimate the effectiveness factor for the reaction at the reactor inlet temperature. The individual pellet may be considered isothermal. The effective diffusion coefficient (called D_{eA} in Froment and Bischoff) for SO_2 in the catalyst pores is about 2.0 $cm^2\ s^{-1}$ at the feed temperature. For a reversible first-order reaction like the one considered here, the generalized Thiele modulus is

$$\phi_{rev} = \phi_{irrev}\sqrt{\frac{1+{k_1}/{k_2}}{{k_1}/{k_2}}}$$

where ϕ_{rev} is the Thiele modulus for the 1st order reversible reaction, ϕ_{irrev} is the usual Thiele modulus for 1st order irreversible reaction, and k_1 and k_2 are the forward and reverse 1st order rate constants for the reaction. (10 points)

(d) Estimate the amount of catalyst and the reactor length (catalyst bed depth) required to produce 10^6 kg/year of SO_3. After allowing for down time, a year of production is 8150 hours. (10 points)

(2) The homogeneous, irreversible, exothermic, liquid phase reaction

$A \rightarrow B$, with rate $r = kC_A$

is to be carried out in a well-mixed reactor. The available reactor has a volume of 1 m^3. It is a simple stirred tank with no provision for heat addition or removal, so it must be run adiabatically. It can be run in batch mode (fill the reactor, run the reaction, drain the reactor, repeat) or in continuous mode (as a CSTR). The available feed stream contains 10 kgmol m^{-3} of species A and none of species B. It is at the ambient temperature of 300 K. It is available in unlimited quantities, so the goal is to process as much of it as possible with the given equipment. The density and specific heat of the feed are 1000 kg m^{-3} and 5 kJ kg^{-1} K^{-1}, respectively. They may be considered independent of temperature and composition. The heat of reaction is -250 kJ mol^{-1}. The rate constant is $2\times10^{10}\exp(-10000/T)$ s^{-1}. It takes 5 minutes to fill the reactor and 10 minutes to drain the reactor.

Helpful hints: $\int \frac{1}{x}\exp\left(\frac{a}{b-x}\right)dx = \mathrm{Ei}\left(\frac{-a}{b-x}\right) - \exp\left(\frac{a}{b}\right)\mathrm{Ei}\left(\frac{-ax}{b(b-x)}\right)$

where Ei(x) is the exponential integral.

The exponential integral may be expressed as the series

$$\mathrm{Ei}(x) = e^{-x}\left(\frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \frac{3!}{x^4} + \frac{4!}{x^5} - \frac{5!}{x^6} + \ldots\right)$$

which converges nicely with just a few terms when abs(x) >> 1.

A table of values of the exponential integral for x from –10 to 10 is attached to the test.

(a) What will be the average reactor throughput (kgmol of feed processed per hour) for each mode of operation (batch and continuous), and which mode of operation is preferable

(i) if we require 60% conversion of A to B (outlet concentrations of 0.4 kgmol m^{-3} A and 0.7 kgmol m^{-3} B)? (10 points)

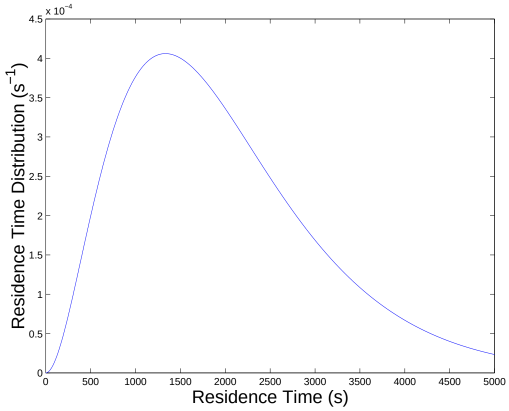
(ii) if we require 99% conversion of A to B (outlet concentrations of 0.01 kgmol m^{-3} A and 1.09 kgmol m^{-3} B)? (10 points)

(b) Based on the above results, it is proposed to run the reactor in continuous (CSTR) mode, with the residence time that, in part a(i), was found to give 60% conversion. Perform a linear stability analysis at the steady state corresponding to 60% conversion. What will happen if we try to run the reactor at these conditions? (15 points)

(c) In an effort to get higher conversion in the continuous mode, the amount of mixing in the reactor was decreased (the impeller used for stirring was run at a slower speed). Under these conditions of high conversion, the reactor can be considered to be isothermal, at the adiabatic reaction temperature. For a feed rate of 0.5 kg s^{-1}, a tracer experiment was performed, and the residence time distribution was measured. It could be fit well by the expression

$$E(\theta) = 1.6875\times10^{-9}\theta^2\exp\left(\frac{-3\theta}{2000}\right)$$

which is plotted below



Predict the outlet concentrations for the partially mixed reactor under these conditions. (15 points)

Values of the exponential integral

x	Ei(*x*)	*x*	Ei(*x*)	*x*	Ei(*x*)	*x*	Ei(*x*)	*x*	Ei(*x*)
-10.0	-2.4922E+03	-5.0	-4.0185E+01	-0.100	1.6228E+00	0.1	1.8229E+00	5.1	1.0213E-03
-9.9	-2.2816E+03	-4.9	-3.7332E+01	-0.096	1.6678E+00	0.2	1.2227E+00	5.2	9.0862E-04
-9.8	-2.0890E+03	-4.8	-3.4698E+01	-0.092	1.7146E+00	0.3	9.0568E-01	5.3	8.0861E-04
-9.7	-1.9130E+03	-4.7	-3.2264E+01	-0.088	1.7632E+00	0.4	7.0238E-01	5.4	7.1980E-04
-9.6	-1.7521E+03	-4.6	-3.0014E+01	-0.084	1.8139E+00	0.5	5.5977E-01	5.5	6.4093E-04
-9.5	-1.6050E+03	-4.5	-2.7934E+01	-0.080	1.8669E+00	0.6	4.5438E-01	5.6	5.7084E-04
-9.4	-1.4705E+03	-4.4	-2.6009E+01	-0.076	1.9223E+00	0.7	3.7377E-01	5.7	5.0855E-04
-9.3	-1.3475E+03	-4.3	-2.4227E+01	-0.072	1.9806E+00	0.8	3.1060E-01	5.8	4.5316E-04
-9.2	-1.2350E+03	-4.2	-2.2577E+01	-0.068	2.0419E+00	0.9	2.6018E-01	5.9	4.0390E-04
-9.1	-1.1320E+03	-4.1	-2.1048E+01	-0.064	2.1066E+00	1.0	2.1938E-01	6.0	3.6008E-04
-9.0	-1.0379E+03	-4.0	-1.9631E+01	-0.060	2.1753E+00	1.1	1.8599E-01	6.1	3.2109E-04
-8.9	-9.5173E+02	-3.9	-1.8316E+01	-0.056	2.2484E+00	1.2	1.5841E-01	6.2	2.8638E-04
-8.8	-8.7289E+02	-3.8	-1.7095E+01	-0.052	2.3266E+00	1.3	1.3545E-01	6.3	2.5547E-04
-8.7	-8.0075E+02	-3.7	-1.5961E+01	-0.048	2.4108E+00	1.4	1.1622E-01	6.4	2.2795E-04
-8.6	-7.3471E+02	-3.6	-1.4906E+01	-0.044	2.5019E+00	1.5	1.0002E-01	6.5	2.0343E-04
-8.5	-6.7426E+02	-3.5	-1.3925E+01	-0.040	2.6013E+00	1.6	8.6308E-02	6.6	1.8158E-04
-8.4	-6.1892E+02	-3.4	-1.3012E+01	-0.036	2.7107E+00	1.7	7.4655E-02	6.7	1.6211E-04
-8.3	-5.6824E+02	-3.3	-1.2161E+01	-0.032	2.8325E+00	1.8	6.4713E-02	6.8	1.4476E-04
-8.2	-5.2183E+02	-3.2	-1.1367E+01	-0.028	2.9701E+00	1.9	5.6204E-02	6.9	1.2928E-04
-8.1	-4.7932E+02	-3.1	-1.0626E+01	-0.024	3.1283E+00	2.0	4.8901E-02	7.0	1.1548E-04
-8.0	-4.4038E+02	-3.0	-9.9338E+00	-0.020	3.3147E+00	2.1	4.2614E-02	7.1	1.0317E-04
-7.9	-4.0470E+02	-2.9	-9.2860E+00	-0.016	3.5419E+00	2.2	3.7191E-02	7.2	9.2188E-05
-7.8	-3.7201E+02	-2.8	-8.6793E+00	-0.012	3.8336E+00	2.3	3.2502E-02	7.3	8.2387E-05
-7.7	-3.4204E+02	-2.7	-8.1103E+00	-0.008	4.2431E+00	2.4	2.8440E-02	7.4	7.3640E-05
-7.6	-3.1457E+02	-2.6	-7.5761E+00	-0.004	4.9402E+00	2.5	2.4915E-02	7.5	6.5831E-05
-7.5	-2.8939E+02	-2.5	-7.0738E+00	0.004	4.9482E+00	2.6	2.1850E-02	7.6	5.8859E-05
-7.4	-2.6630E+02	-2.4	-6.6007E+00	0.008	4.2591E+00	2.7	1.9182E-02	7.7	5.2633E-05
-7.3	-2.4512E+02	-2.3	-6.1544E+00	0.012	3.8576E+00	2.8	1.6855E-02	7.8	4.7072E-05
-7.2	-2.2569E+02	-2.2	-5.7326E+00	0.016	3.5739E+00	2.9	1.4824E-02	7.9	4.2104E-05
-7.1	-2.0786E+02	-2.1	-5.3332E+00	0.020	3.3547E+00	3.0	1.3048E-02	8.0	3.7666E-05
-7.0	-1.9150E+02	-2.0	-4.9542E+00	0.024	3.1763E+00	3.1	1.1494E-02	8.1	3.3700E-05
-6.9	-1.7649E+02	-1.9	-4.5937E+00	0.028	3.0261E+00	3.2	1.0133E-02	8.2	3.0155E-05
-6.8	-1.6271E+02	-1.8	-4.2499E+00	0.032	2.8965E+00	3.3	8.9390E-03	8.3	2.6986E-05
-6.7	-1.5005E+02	-1.7	-3.9210E+00	0.036	2.7827E+00	3.4	7.8910E-03	8.4	2.4154E-05
-6.6	-1.3843E+02	-1.6	-3.6053E+00	0.040	2.6813E+00	3.5	6.9701E-03	8.5	2.1621E-05
-6.5	-1.2775E+02	-1.5	-3.3013E+00	0.044	2.5899E+00	3.6	6.1604E-03	8.6	1.9356E-05
-6.4	-1.1793E+02	-1.4	-3.0072E+00	0.048	2.5068E+00	3.7	5.4478E-03	8.7	1.7331E-05
-6.3	-1.0892E+02	-1.3	-2.7214E+00	0.052	2.4306E+00	3.8	4.8202E-03	8.8	1.5519E-05
-6.2	-1.0063E+02	-1.2	-2.4421E+00	0.056	2.3604E+00	3.9	4.2671E-03	8.9	1.3898E-05
-6.1	-9.3002E+01	-1.1	-2.1674E+00	0.060	2.2953E+00	4.0	3.7794E-03	9.0	1.2447E-05
-6.0	-8.5990E+01	-1.0	-1.8951E+00	0.064	2.2346E+00	4.1	3.3489E-03	9.1	1.1150E-05
-5.9	-7.9538E+01	-0.9	-1.6228E+00	0.068	2.1779E+00	4.2	2.9688E-03	9.2	9.9881E-06
-5.8	-7.3601E+01	-0.8	-1.3474E+00	0.072	2.1246E+00	4.3	2.6329E-03	9.3	8.9485E-06
-5.7	-6.8135E+01	-0.7	-1.0649E+00	0.076	2.0744E+00	4.4	2.3360E-03	9.4	8.0179E-06
-5.6	-6.3102E+01	-0.6	-7.6988E-01	0.080	2.0269E+00	4.5	2.0734E-03	9.5	7.1848E-06
-5.5	-5.8466E+01	-0.5	-4.5422E-01	0.084	1.9820E+00	4.6	1.8410E-03	9.6	6.4388E-06
-5.4	-5.4193E+01	-0.4	-1.0477E-01	0.088	1.9393E+00	4.7	1.6352E-03	9.7	5.7709E-06
-5.3	-5.0256E+01	-0.3	3.0267E-01	0.092	1.8987E+00	4.8	1.4530E-03	9.8	5.1727E-06
-5.2	-4.6625E+01	-0.2	8.2176E-01	0.096	1.8599E+00	4.9	1.2915E-03	9.9	4.6369E-06
-5.1	-4.3276E+01	-0.1	1.6228E+00	0.100	1.8229E+00	5.0	1.1483E-03	10.0	4.1570E-06

Some useful indefinite integrals
(from the CRC handbook of Chemistry and Physics)

517. $\int e^x \, dx = e^x$

518. $\int e^{-x} \, dx = -e^{-x}$

519. $\int e^{ax} \, dx = \frac{e^{ax}}{a}$

520. $\int x \, e^{ax} \, dx = \frac{e^{ax}}{a^2}(ax - 1)$

521. $$\int x^m e^{ax} \, dx = \begin{cases} \dfrac{x^m e^{ax}}{a} - \dfrac{m}{a} \displaystyle\int x^{m-1} e^{ax} \, dx \\ \text{or} \\ e^{ax} \displaystyle\sum_{r=0}^{m} (-1)^r \dfrac{m! x^{m-r}}{(m-r)! a^{r+1}} \end{cases}$$

522. $\int \frac{e^{ax} \, dx}{x} = \log x + \frac{ax}{1!} + \frac{a^2 x^2}{2 \cdot 2!} + \frac{a^3 x^3}{3 \cdot 3!} + \cdots$

523. $\int \frac{e^{ax}}{x^m} \, dx = -\frac{1}{m-1} \frac{e^{ax}}{x^{m-1}} + \frac{a}{m-1} \int \frac{e^{ax}}{x^{m-1}} \, dx$

524. $\int e^{ax} \log x \, dx = \frac{e^{ax} \log x}{a} - \frac{1}{a} \int \frac{e^{ax}}{x} \, dx$

525. $\int \frac{dx}{1 + e^x} = x - \log(1 + e^x) = \log \frac{e^x}{1 + e^x}$

526. $\int \frac{dx}{a + be^{px}} = \frac{x}{a} - \frac{1}{ap} \log(a + be^{px})$

527. $\int \frac{dx}{ae^{mx} + be^{-mx}} = \frac{1}{m\sqrt{ab}} \tan^{-1}\left(e^{mx}\sqrt{\frac{a}{b}}\right), \qquad (a > 0, b > 0)$

528. $$\int \frac{dx}{ae^{mx} - be^{-mx}} = \begin{cases} \dfrac{1}{2m\sqrt{ab}} \log \dfrac{\sqrt{a}\, e^{mx} - \sqrt{b}}{\sqrt{a}\, e^{mx} + \sqrt{b}} \\ \text{or} \\ \dfrac{-1}{m\sqrt{ab}} \tanh^{-1}\left(\sqrt{\dfrac{a}{b}}\, e^{mx}\right), \qquad (a > 0, b > 0) \end{cases}$$