Name__________________________ Student Number _____________

University of Toronto
Faculty of Applied Science and Engineering
Final Examination, December 21, 2001
CHE412F - Advanced Chemical Reaction Engineering
Examiner: B.A. Saville

Questions 1 to 4 are worth 25 marks each
Exam total = 100

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1. A kinetics study of a gas-solid reaction A(g) + bB(s) → products was conducted with 1.0mm (dia) spherical particles at 525°C and 3 bar. 100% conversion of the particles was obtained after 4.0 min., with surface reaction control.
   a) A second study was conducted with 2.0mm particles at 1 bar and 675°C. The same time for complete reaction was obtained. What is the activation energy for this process, assuming surface reaction control?
   b) A further increase in particle size was contemplated, to 5.0mm, but it was expected that this would change to the process to one controlled by ash-layer diffusion. Design/describe a set of experiments that could be performed to check for such a change in the rate-limiting step. Indicate what should be measured, appropriate conditions, and the type of information that could be obtained from each (set of) experiment(s).
   c) A conveyor system was set up to process a solids feed stream consisting of 40% 1.0mm particles and 60% 2.0mm particles at the same conditions specified in part (a). Determine the overall fractional conversion when 75% of the 2.0mm particles have been converted.

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2. A careless researcher spilled 200mL of a dangerous, volatile liquid in a chemical processing facility, and, while the building was evacuated, the HAZMAT team was called in. They arrived on the scene within 5 minutes, armed with their MSDS manual and full protective gear (white suits, self-contained breathing apparatus, etc.). The building engineer advised them that there was normally some "stratification" of the building air, producing approximately 4 reasonably well-mixed zones in the building. The spill took place in the first zone, where a fumehood was removing about 15 m^3 of air per minute. Air that was not removed via the fumehood could be expected to travel from zone 1 to zone 4, where it would be removed via the building's normal ventilation system at 5 m^3 per minute. The MSDS indicated that the liquid density was 0.7 g/mL, with an ambient vapor pressure of 85 kPa and an evaporation rate of about 400 mL/min. The molar mass of the liquid was 76 g/mol. Its threshold limit value (TLV) indicates that the compound would be toxic at a concentration of 10 parts per million (volume basis). The ambient temperature and pressure in the building are 23°C and 100kPa, respectively. The building is 6m high, 15m wide, and 40 m long.
   a) Set up material balance relationships that would allow you to calculate the concentration versus time profiles in the four compartments.
   b) If it took one minute to evacuate zone 1, what is the likelihood that workers in that area were exposed to toxic levels of the compound?
   c) If the spill area had been isolated, so that none of the contaminated air migrated into zone 2 (and beyond), and the only means of removal was via the fumehood, how long would it take for the concentration in zone 1 fall below the TLV?

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3. A tracer study was conducted to examine mixing in a bubble column reactor by pulse injection of a tracer gas into the bottom of the column. The following data were acquired:

Time, s	5	10	20	35	45	65	95	140	170
Conc, dimensionless	0.0	1.0	5.6	10.0	8.8	4.8	1.7	0.2	0.0

a) Determine the mean residence time and N for this system
b) Use your model parameters to predict the concentration at 35s. Use only integer values of N.

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4. You are to select and design a reactor for a gas-liquid reaction A(g) + bB(ℓ) → products. A previous kinetics study has established the rate constants for the process, under a variety of operating conditions. The gaseous feed to the system is made up of 10% A, and the balance is an inert.

   a) Under condition set #1, it has been established that the reaction takes place mainly in the bulk liquid.
      (i) Sketch the concentration profile for A and B across the bulk gas, liquid film, and bulk liquid, assuming that the two film model is valid. Carefully label the regions and all profiles.
      (ii) What type of reactor and related process equipment would be most appropriate for the reaction under these conditions? Justify your answer.

   b) Under condition set #2, at a somewhat higher temperature, it has been established that the Hatta number for the process is approximately 22.
      (i) Sketch the concentration profile for A and B across the bulk gas, liquid film, and bulk liquid, assuming that the two film model is valid. Carefully label the regions and all profiles.
      (ii) What type of reactor and related process equipment would be most appropriate for the reaction under these conditions? Justify your answer.
      (iii) Estimate the value of N_A at the transition from the liquid film to the bulk liquid (i.e., at z = 1)?

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5. **Bonus questions: 5 marks each**
    a) Explain why the segregated flow model is an appropriate mixing model to assess the performance of a non-catalytic gas-solid reactor
    b) List 4 important characteristics of an ideal tracer

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Table 9.1 SCM: Summary of $t(f_B)$ for various shapes of particle[1]

Particle shape	Size parameters	f_B (size parameters)	$t(f_B)$
flat plate (one face permeable)	length l (of zone unreacted) L (of particle)	$1 - \frac{l}{L}$	$\frac{\rho_{Bm} L f_B}{b c_{Ag}} \left(\frac{1}{k_{Ag}} + \frac{L f_B}{2 D_e} + \frac{1}{k_{As}} \right)$
cylinder (ends sealed)	radius r_c (of core unreacted) R (of particle)	$1 - \left(\frac{r_c}{R}\right)^2$	$\frac{\rho_{Bm} R}{b c_{Ag}} \left\{ \frac{f_B}{2 k_{Ag}} + \frac{R}{4 D_e} \left[f_B + (1 - f_B)\ln(1 - f_B) \right] + \frac{1}{k_{As}} \left[1 - (1 - f_B)^{1/2} \right] \right\}$
sphere	same as for cylinder	$1 - \left(\frac{r_c}{R}\right)^3$	$\frac{\rho_{Bm} R}{b c_{Ag}} \left\{ \frac{f_B}{3 k_{Ag}} + \frac{R}{6 D_e} \left[1 - 3(1 - f_B)^{2/3} + 2(1 - f_B) \right] + \frac{1}{k_{As}} \left[1 - (1 - f_B)^{1/3} \right] \right\}$ (9.1-28)

[1] Reaction: $A(g) + bB(s) \rightarrow$ products $[(s),(g)]$; first order with respect to A at core surface.
Particle(B): constant-size (L, R constant); isothermal.
For t_1 (time for complete reaction of particle), set $f_B = 1$; $[(1 - f_B)\ln(1 - f_B) \rightarrow 0]$.
Symbols: see text and Nomenclature.