04-CHEM-A4, CHEMICAL REACTOR ENGINEERING

MAY 2015

3 hours Duration

1. If doubt exists as to the interpretation of any question, please submit with your answer a clear statement of any assumption(s) you make. If possible, please underline or enclose any such statement in a box.

2. This is an OPEN BOOK EXAM. You may bring to this exam

   - the official designated textbook by Fogler – any edition – annotated in margins, etc. as desired. No loose notes allowed.
   - your own unit conversion tables and/or mathematical tables such as a CRC Handbook.
   - a non-communicating, programmable electronic calculator using a small operating guide. Please write the name and model of your calculator on the first inside left-hand sheet of the exam workbook.

3. Graph paper will be provided.

4. Any **four** questions constitute a complete paper and, unless you indicate otherwise, only the first four answers as they appear in your answer booklet will be marked.

5. Each question is worth 20 points. Marking schemes are provided in brackets after each question.

6. Technical content is the key ingredient in your answers. However, no credit will be given for deriving rate expressions, or standard formulas that are available in the textbook. Clear writing is essential, particularly when explanations are required.

7. It will help the examiner if you could cite the origin of significant formula used – e.g., Fogler, eq. (3-44).

Marking Scheme – Four questions comprise a complete exam.

1. 20 points
2. 20 points
3. 20 points – a) 10 points, b) 10 points
4. 20 points
5. 20 points

Ethyl acetate ($CH_3COOC_2H_5$) is to be manufactured by the esterification of acetic acid (CH_3COOH) with ethanol (C_2H_5OH) in an isothermal batch reactor as shown below:

$$CH_3COOH\ (\mathbf{A}) + C_2H_5OH\ (\mathbf{B}) = CH_3COOC_2H_5\ (\mathbf{C}) + H_2O\ (\mathbf{D})$$

A production rate of 10,000 kg/day of ethyl acetate is required. The reactor will be charged with a mixture containing 500 kg/m^3 ethanol, 250 kg/m^3 acetic acid, the remainder being water, and very small quantity of hydrochloric acid as a catalyst. The density of this mixture is 1045 kg/m^3, which will be assumed constant throughout the reaction. The reaction is reversible with a rate equation given by

$$r_A = k_f\, C_A\, C_B - k_r\, C_C\, C_D$$

At the operating temperature of 100 °C, the rate constants have the following values:

$$k_f = 8 \times 10^{-6}\ m^3/kmol.s$$

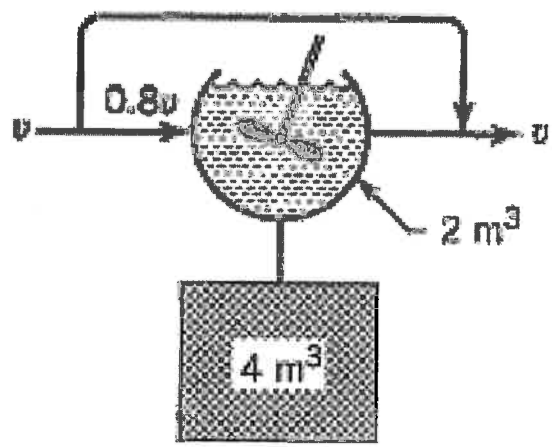
$$k_r = 2.7 \times 10^{-6}\ m^3/kmol.s$$

The reaction mixture will be discharged when the conversion of acetic acid is 30%. A time of 30 minutes is required for discharging, cleaning, and recharging. Determine the volume of reactor required.

The second order aqueous reaction

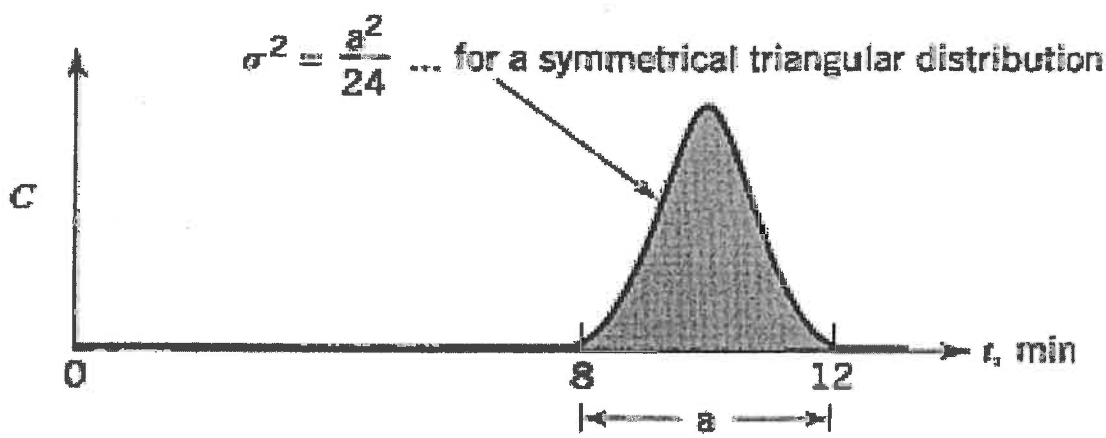
$$A + B \rightarrow R + S$$

is run in a large tank reactor ($V = 6\ m^3$) and for an equimolar food stream ($C_{A0} = C_{B0}$) conversion of reactants is 60%. Unfortunately, agitation in the reactor is rather inadequate and tracer tests of the flow within the reactor give the flow model shown below which includes a 4 m^3 dead zone:



What size of mixed flow reactor will equal the performance of the unit shown?

Calculations show that a plug flow reactor would give 99.9% conversion of reactant, which is in aqueous solution. However, the reactor has a residence time distribution as shown in the figure below:



The variance for a symmetrical triangle with base "a" rotating about its centre of gravity is given by $\sigma^2 = a^2/24$

(a) If C_{A0} = 1000, what outlet concentration can we expect in the reactor for a first order reaction?

(b) Repeat part (a) using the tanks-in-series model.

Laboratory experiments on an irreversible, homogeneous gas-phase reaction

$$2A + B \rightarrow 2C$$

have shown the reaction rate constant to be 1 x 10^5 $L^2/mol^2.s$ at 500 °C. Analysis of isothermal data from this reaction has indicated that a rate expression of the form

$$-r_A = kC_A C_B^2$$

provides an adequate representation for the data at 500 °C and 1 atm total pressure. Calculate the volume of an isothermal, isobaric plug-glow reactor that would be required to process 6 L/s of a feed gas containing 25% A, 25 % B, and 50% inerts by volume for a fractional conversion of 90% of component A.

Kinetic experiments on the solid catalyzed reaction

$$A \rightarrow 3R$$

are conducted at 8 atm and 700 °C in a mixed reactor 960 cm^3 in volume and containing 1 gram of catalyst of diameter d_p = 3 mm. Feed consisting of pure A is introduced at various rates into the reactor and the partial pressure of A in the exit stream is measured for each feed rate as shown below:

Volumetric Feed Rate, V_0 (in liters per hour)	Partial Pressure $p_{A,out}/p_{A,in}$
100	0.8
22	0.5
4	0.2
1	0.1
0.6	0.05

Find a rate equation to represent the rate of reaction on catalyst of this size.

The Periodic Table of the Elements

- [ ] Alkali metals
- [ ] Alkaline earth metals
- [ ] Transition metals
- [ ] Other metals
- [ ] Metalloids (semi-metal)
- [ ] Nonmetals
- [ ] Halogens
- [ ] Noble gases

Element name → Mercury
Atomic # → 80
Symbol → Hg
Avg. Mass → 200.59

1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Hydrogen 1 **H** 1.01																		Helium 2 **He** 4.00
Lithium 3 **Li** 6.94	Beryllium 4 **Be** 9.01												Boron 5 **B** 10.81	Carbon 6 **C** 12.01	Nitrogen 7 **N** 14.01	Oxygen 8 **O** 16.00	Fluorine 9 **F** 19.00	Neon 10 **Ne** 20.18
Sodium 11 **Na** 22.99	Magnesium 12 **Mg** 24.31												Aluminum 13 **Al** 26.98	Silicon 14 **Si** 28.09	Phosphorus 15 **P** 30.97	Sulfur 16 **S** 32.07	Chlorine 17 **Cl** 35.45	Argon 18 **Ar** 39.95
Potassium 19 **K** 39.10	Calcium 20 **Ca** 40.08		Scandium 21 **Sc** 44.96	Titanium 22 **Ti** 47.88	Vanadium 23 **V** 50.94	Chromium 24 **Cr** 52.00	Manganese 25 **Mn** 54.94	Iron 26 **Fe** 55.85	Cobalt 27 **Co** 58.93	Nickel 28 **Ni** 58.69	Copper 29 **Cu** 63.55	Zinc 30 **Zn** 65.39	Gallium 31 **Ga** 69.72	Germanium 32 **Ge** 72.61	Arsenic 33 **As** 74.92	Selenium 34 **Se** 78.96	Bromine 35 **Br** 79.90	Krypton 36 **Kr** 83.80
Rubidium 37 **Rb** 85.47	Strontium 38 **Sr** 87.62		Yttrium 39 **Y** 88.91	Zirconium 40 **Zr** 91.22	Niobium 41 **Nb** 92.91	Molybdenum 42 **Mo** 95.94	Technetium 43 **Tc** (98)	Ruthenium 44 **Ru** 101.07	Rhodium 45 **Rh** 102.91	Palladium 46 **Pd** 106.42	Silver 47 **Ag** 107.87	Cadmium 48 **Cd** 112.41	Indium 49 **In** 114.82	Tin 50 **Sn** 118.71	Antimony 51 **Sb** 121.76	Tellurium 52 **Te** 127.60	Iodine 53 **I** 126.90	Xenon 54 **Xe** 131.29
Cesium 55 **Cs** 132.91	Barium 56 **Ba** 137.33	57-70 *	Lutetium 71 **Lu** 174.97	Hafnium 72 **Hf** 178.49	Tantalum 73 **Ta** 180.95	Tungsten 74 **W** 183.84	Rhenium 75 **Re** 186.21	Osmium 76 **Os** 190.23	Iridium 77 **Ir** 192.22	Platinum 78 **Pt** 195.08	Gold 79 **Au** 196.97	Mercury 80 **Hg** 200.59	Thallium 81 **Tl** 204.38	Lead 82 **Pb** 207.20	Bismuth 83 **Bi** 208.98	Polonium 84 **Po** (209)	Astatine 85 **At** (210)	Radon 86 **Rn** (222)
Francium 87 **Fr** (223)	Radium 88 **Ra** (226)	89-102 **	Lawrencium 103 **Lr** (262)	Rutherfordium 104 **Rf** (267)	Dubnium 105 **Db** (268)	Seaborgium 106 **Sg** (271)	Bohrium 107 **Bh** (272)	Hassium 108 **Hs** (270)	Meitnerium 109 **Mt** (276)	Darmstadtium 110 **Ds** (281)	Roentgenium 111 **Rg** (280)	Copernicium 112 **Cn** (285)	Ununtrium 113 **Uut** (284)	Ununquadium 114 **Uuq** (289)	Ununpentium 115 **Uup** (288)	Ununhexium 116 **Uuh** (293)	Ununseptium 117 **Uus** (294?)	Ununoctium 118 **Uuo** (294)

*lanthanides	Lanthanum 57 **La** 138.91	Cerium 58 **Ce** 140.12	Praseodymium 59 **Pr** 140.91	Neodymium 60 **Nd** 144.24	Promethium 61 **Pm** (145)	Samarium 62 **Sm** 150.36	Europium 63 **Eu** 151.97	Gadolinium 64 **Gd** 157.25	Terbium 65 **Tb** 158.93	Dysprosium 66 **Dy** 162.50	Holmium 67 **Ho** 164.93	Erbium 68 **Er** 167.26	Thulium 69 **Tm** 168.93	Ytterbium 70 **Yb** 173.04
**actinides	Actinium 89 **Ac** (227)	Thorium 90 **Th** 232.04	Protactinium 91 **Pa** 231.04	Uranium 92 **U** 238.03	Neptunium 93 **Np** (237)	Plutonium 94 **Pu** (244)	Americium 95 **Am** (243)	Curium 96 **Cm** (247)	Berkelium 97 **Bk** (247)	Californium 98 **Cf** (251)	Einsteinium 99 **Es** (252)	Fermium 100 **Fm** (257)	Mendelevium 101 **Md** (258)	Nobelium 102 **No** (259)