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UPES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination - April, 2018

Program/Course : B. Tech Chemical (Spl. in Refining and Petrochemicals)
Subject: Process Modelling and Simulation
Code: CHEG439
No. of pages: 2

Semester: VIII
Max. Marks: 100
Duration: 3 hrs

NOTE:

(A) **OPEN BOOK and OPEN NOTES EXAMINATION**

(B) Assume all missing data. **State your assumptions clearly.** Sketch wherever necessary.

SECTION - A **ANSWER ALL QUESTIONS** $30 \times 2 = 60$ marks

1. Some of the condensation reactions that take place when formaldehyde (F) is added to sodium paraphenolsulfonate (M) in an alkaline-aqueous solution have been studied. It was found that the reactions could be represented by the following equations:

$F + M \rightarrow MA,$	$k_1 = 0.15$ L/gmol min
$F + MA \rightarrow MDA,$	$k_2 = 0.49$
$MA + MDA \rightarrow DDA,$	$k_3 = 0.14$
$M + MDA \rightarrow DA,$	$k_4 = 0.14$
$MA + MA \rightarrow DA,$	$k_5 = 0.04$
$MA + M \rightarrow D,$	$k_6 = 0.056$
$F + D \rightarrow DA,$	$k_7 = 0.50$
$F + DA \rightarrow DDA,$	$k_8 = 0.50$

where M, MA, and MDA are monomers and D, DA, and DDA are dimers. The process continues to form trimers. The rate constants were evaluated using the assumption that the molecularity of each reaction was identical to its stoichiometry. Derive a dynamic model for these reactions taking place in a single, isothermal CSTR. Carefully define your terms and list your assumptions. [20 marks] CO 1 CO 2 & CO 3

Also, write a computer code to solve the model equations derived for the above said CSTR system. [10 marks] CO 5

2. Coupled first-order equations arise fre- quently in chemical engineering, where there are two dependent variables and their dynamics are coupled through the nonlinear functions. Apply this to a CSTR experiencing a slow catalyst decay, so that the deactivation rate is proportional to the reactant concentration (parallel deactivation). Let x be the reactant concentration and y be the catalyst activity. The reaction rate is represented by the product xy and the rate of catalyst decay is given by ϵxy with $\epsilon << 1$, which is taken to be slower than the main reaction rate. Derive the mass balance equations also mention the initial conditions necessary for numerical integration. [15 marks] CO 1 CO 2 & CO 3

Also, write a computer code to solve the model equations derived for the above said CSTR system. [15 marks] CO 5

SECTION - B **ANSWER ANY ONE QUESTION** $40 \times 1 = 40$ marks

1. Fast pyrolysis, the rapid heating of biomass in the oxygen-free atmosphere, has been considered as a promising technology for the production of transportation fuels, speciality and fine chemicals, and furnace and boiler fuel. Catalytic fast pyrolysis (CFP) has a potential option for improving the quality of organic products from fast pyrolysis of biomass. The lab-scale reactor of pyrolysis vapours upgrading was performed in either a fixed bed or fluidised bed reactors. In comparison with fixed bed reactor, fluidised bed operations could be preferred because it produces relatively lesser coke and thus reduces catalyst deactivation. The pyrolysis vapours upgrading in fluidised bed follows a similar procedure in the petroleum industry with the reactor concept of fluid catalytic cracking (FCC). In a typical FCC unit, catalyst from the regenerator enters at the bottom of the riser where it reacts with the feed in the riser and is separated from the gaseous products by the cyclone. The catalyst flows back to the regenerator where the air is injected to burn off the coke that is deposited on the active surface of the catalyst.

   Deduce from the first principles, the model equations representing the prediction of catalyst residence time in the riser is performed for studying the contact time of vapours with the catalyst. This is examined by the effect of catalyst feed rate and gas flow rate on the hydrodynamic behaviour and catalyst residence time distribution (RTD).

   CO 3 & CO 4

   Ref. Numerical simulation of catalytic upgrading of biomass pyrolysis vapours in a FCC riser, Fuel Processing Technology 171 (2018) 162 - 172.

2. Consider the elementary gas phase reaction

$$\mathrm{A} + \mathrm{B} \underset{\mathrm{k_2}}{\overset{\mathrm{k_1}}{\rightleftharpoons}} \mathrm{R} \tag{1}$$

   which takes place in a non-isothermal plug flow reactor. Set up the differential equations which can be used to find the length of the reactor for a feed consisting of A, B, R and inert gas. Assume that the values of k_1 and k_2, are known. If k(s) are unknown, suggest two experimental methods to obtain them. **Do not assume that the velocity in the axial direction is constant.** CO 3 & CO 4