1) Catalytic cracking of a hydrocarbon (A) to form desired product B is being conducted in a moving-bed reactor under certain conditions. While the desired product is formed, a parallel reaction A → C occurs simultaneously to form an undesired product *C*. Both reactions are known to be represented by a second-order rate law. Rate constants for these two reactions, respectively are k_1 and k_2. Relevant systematic experimentation suggests that the catalytic deactivation is not affected by the gas-phase concentration. Moreover, these experiments suggested that the deactivation follows a first-order decay law; k_d being the corresponding decay constant. The feed stream is being constantly diluted with an inert gas in such a way that the volume changes can be neglected with reaction. The reactant feed stream flows rapidly through the reactor when compared with the flow of the catalysts through the reactor. Assuming the weight of the catalyst to be W and that the catalyst moves within the bed with a mass flow rate of F, hydrocarbon feed gas stream is fed into the reactor at the inlet with a molar flow rate of u and a concentration of C_0,
   a) Write a model to capture to the activity as a function of W, F and other parameters.
   b) Find the relationship between the conversion of species A and other parameters.

2) Consider a single-step first-order heterogenous reaction A(g) → B. Reaction was conducted using catalyst spherical pellets of two different sizes (with all other conditions being same) and the rate of reaction was measured. The reaction rates for different sizes are in Table 1. Assume that the external mass transfer resistances are negligible.

Table 1: Rate of reaction at different particle radius

	Radius (mm)	Rate $(-r'_{obs})$ (mol/gcat/min)
1	15	0.002
2	2	0.009

   a) Find the effectiveness factor and Thiele modulus for each pellet.
   b) Identify whether the reaction is conducted under internal diffusion or reaction limiting conditions.

3) In case of multiple reactions conducted under diffusional limitations, identification and quantification of diffusional effects on the selectivity ratio is very important. Consider the simplest case of two parallel, independent reactions A→B with order n_1 and C→D with order n_2
   a) Find the selectivity ratio under strong pore diffusional limitations for this system.
   b) If the diffusivity of species B and C are equal and $n_1=n_2=1$, compare the selectivity ratios with and without diffusional limitations and discuss the diffusional effects on the selectivity.

4) Consider a fluid-solid reaction A(g) + bB(s) → solid products that can be modelled using a shrinking core model of unchanging size. Assume the surface reaction to be first-order. Assuming the core to be a flat plate of half thickness of *L*, find the conversion as a function of time under
   I. Film diffusion controlling
   II. Ash-layer controlling
   III. Reaction controlling

5) Repeat question (4) by assuming the core to be a cylinder with radius r_c,

6) A catalytic reaction is being conducted in a fixed-bed reactor. In order to determine the residence-time distribution, a pulse-tracer experiment was performed. Octadecane tagged with carbon-14 was used as a liquid tracer and was injected into the reactor feed stream at the inlet. Samples of the reactor effluent were collected at regular time intervals following injection of the tracer and the concentration of the carbon-14 tracer was analysed. The tracer concentration in the reactor effluent as a function of time is in Table 2. Find E-curve, mean residence time t_m, and the variance of the E-curve σ.

Table 2: Tracer relative concentration in the effluent

Time (mins)	Relative concentration	Time (mins)	Relative concentration
2.50	37.5	11.50	400
3.75	51	13.50	315
4.00	110	14.25	237
5.00	184	16.00	275
5.30	285	18.75	184
6.50	337.5	21.50	131.2
7.00	397	23.25	86.5
7.50	428	27.5	73
8.75	431	30.00	37.5
10.00	425	35.00	25

7) Consider a reactor whose residence-time distribution is given by that in question (6). Suppose that the reaction conducted in the reactor is a first-order (or pseudo-first order) reaction.
   a) If the reactor were to be completely segregated, find the rate constant k if the conversion were to be 90%?
   b) Find the reactor contacting efficiency
      $\eta = 100 * t_m / t_p$
      where, t_m is the mean residence time of the reactor, t_p is the mean residence time of the plug flow reactor in which same reaction with same kinetics is conducted up to the same conversion as that observed in (b).

8) The following data is given for a reactive gas –liquid system, in which the following reaction takes place: $A(g) + 2B(l) = C(l)$. $C_A^* = 1 \times 10^{-5}$ mol/cm^3, $C_{B0}=2 \times 10^{-3}$ mol/cm^3, $D_A=D_B =1 \times 10^{-5}$ cm^2/s, Liquid phase mass transfer coefficient $k_L = 2 \times 10^{-3}$ cm/s, Reaction rate constant k = 2×10^6 cm^3/mol.s. The liquid phase reaction is known to be first order in both reactants and it may be considered fast enough for the bulk concentration of A to be rendered zero. Find the value of the flux of absorption of A (N_A) from the gas into the liquid phase. Report clearly the values of q and $\sqrt{M}$. If C_{B0} is doubled, by what factor does the rate go up ?

9) Given below are the results of experiments conducted on a reactive gas (A)-liquid (B) system (the reaction stoichiometry requires one mole of B per mole of A). The data on the flux (N_A) versus the liquid phase reagent concentration (C_{B0}) is given in the following table.

N_A (mol/cm^{2}s)	C_{B0} (mol/m^3)
2.75×10^{-7}	1×10^{-3}
3.89×10^{-7}	2×10^{-3}
5.00×10^{-7}	3×10^{-3}
5.50×10^{-7}	4×10^{-3}
6.30×10^{-7}	5×10^{-3}

It is given that $k_L = 5 \times 10^{-3}$ cm/s, $C^*_A = 2 \times 10^{-5}$ mol/cm^3, $D_A = D_B = 1 \times 10^{-5}$ cm^2/s and that the parameter $\hat{a}\delta \ll 1$. It is also known that the reaction is first order in both A and B. Using ALL the above data find the `best' value of the second order rate constant.

The same reaction is carried out in a different reactor for $C_{B0} = 1 \times 10^{-3}$ mol/cm^3. The value of k_L in the new reactor is given as 7.5×10^{-2} cm/s. The measured rate is given by 15×10^{-7} mol/cm^{2}s. Can the value of the rate constant be determined from this data point? If yes, what is the value and how does it compare with the one determined above and if not, then explain why not.

10) The oxidation of sodium dithionite in aqueous alkaline solution by oxygen from the gas phase is a reaction often used in the mass transfer – characterization of reacting equipment. Under appropriate conditions, the reaction is zero order in oxygen and first order in sodium dithionite concentration. The stoichiometry requires one mole of oxygen for every mole of sodium dithionite. Consider this reaction being carried out at 308 K in a batch stirred vessel with continuous flow of the gas. The rate constant at 308 K is 8 s^{-1}. Assume the diffusivities of the gas and liquid phase reactants to be equal at 2×10^{-9} m^2/s, and the value of A* under the conditions employed to be 1×10^{-3} kmol/m^3. The initial concentration of the dithionite is 0.06 kmol/m^3. The liquid is well mixed.

  a. Assuming k^0_L values to be typically of the order of 0.02 - 0.04 cm/s., what would be a 'safe' concentration of dithionite above which the reaction may be considered to take place in the fast reaction regime? Solute depletion in the gas phase is negligible.

  b. Derive an equation for the concentration of sodium dithionite in the liquid as a function of time. (iii) Under the above conditions, if an interfacial area (per unit volume of the liquid) of 2.5 cm^{-1} is available in the vessel, what is the time required for the concentration calculated in (i) above to be reached? If the experiment is continued beyond this time, sketch the variation of dissolved oxygen with time in the experiment.

  c. Under the above conditions, if an interfacial area (per unit volume of the liquid) of 2.5 cm^{-1} is available in the vessel, what is the time required for the concentration calculated in (a) above to be reached? If the experiment is continued beyond this time, sketch the variation of dissolved oxygen with time in the experiment.

11) Formulate the film theory differential equation for a reaction that is pseudo-zero order, (i.e.,

zero order in A and a flat profile of c_B throughout the film) in the fast regime. Solve the equation to obtain the enhancement factor in terms of an appropriately defined Hatta parameter.

12) For a gas phase reaction *A* going to *B* performed in a spinning basket reactor, following data is obtained

Temperature (^{0}C)	227	227	237
Total molar feed rate (mol/min)	1	4	9
Conversion	0.8	0.6	0.9

The catalyst loading is 50gm and the operating pressure is 8 atm.

a. Calculate apparent activation energy and apparent order of the reaction.
b. Calculate the true activation energy and order.
c. Calculate the effectiveness factor at the total molar flow rate of 1 mol/min.

13) A first order liquid phase reaction is performed in a reactor that behaves almost like an ideal CSTR in laboratory. The residence time of the CSTR is 3.3 min and the conversion obtained is 50%.
The same reaction is to be performed in a tubular reactor. The results of a tracer injection RTD studies performed on this tubular reactor gives the following results:

time	0	2	5	8	10	13	16	18	20
C (t) mg/lit	0	2.5	6	12	15	12	7	3	0

Find the conversion using closed vessel dispersion model, tank-in-series model, ideal CSTR model and ideal PFR model.

14) A first order isomerization reaction with intrinsic rate constant of 0.1 min^{-1} is taking place in a packed tubular reactor of 200 cm length and 8 cm diameter. The feed flow rate of pure reactant is 10 mol/min the conversion obtained is 0.6. The non-catalytic packing is replaced with new packing of smaller size so that the standard deviation in the E curve is reduced by half. Calculate the new conversion. The molar density of the reaction mixture may be assumed as 10 mol/lit.

15) For a reaction *A + B = C* on heterogeneous catalyst, following are the observations made in the laboratory experiment with a differential reactor. Interpret these observations and propose an adsorption based reaction mechanism.
    i) If we send pure *C* to the reactor, the product stream is pure *C*
    ii) Reaction rate is highly sensitive to change in temperature.
    iii) For very low partial pressure of *A* in the feed, the reaction rate increases linearly with increase in partial pressure of *A* at constant partial pressure of *B*, and under otherwise similar conditions.
    iv) For higher concentration of *A* in the feed, the reaction rate is independent of partial of *A* at constant partial pressure of *B*, and under otherwise similar conditions.

    v) Reaction rate is independent of concentration of *C* in the feed.
    vi) Reaction rate increases linearly with increase in partial pressure of *B* at constant partial pressure of *A*, and under otherwise similar conditions.

16) For the reaction A + 3B = C, derive the rate equation if the surface reaction controls the overall rate. Given: *A* adsorbs on 3 sites whereas *B* and *C* adsorb on single sites each.

17) For the reaction A + B = C + D (reversible) derive the rate equation if
    i) Surface reaction controls

    ii) Adsorption of B controls

    iii) Desorption of C controls

    In the following cases:

    a. All the components adsorb on the catalyst

    b. Adsorption of *A* and *D* are negligible

    c. There are two types of sites on the catalyst; *A* and *B* adsorb on one type and *C* and *D* adsorb on the other.

18) Derive the expression for the conversion obtained in a tubular reactor approximated as series of *n* CSTRs.

19) Derive the equation for the Thiele Modulus in case of catalysts with following shapes:
    a) Cylindrical: The circular faces are non-catalytic and diffusion occurs only through the lateral face.
    b) A cylindrical channel (or pore) with catalyst coated on the wall from inside.
    c) A slab: Diffusion occurs only through the two opposite large faces