

# INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

Mid-Autumn Semester Examination 2023-24

Subject Name: Computer aided Process Engineering

Full Marks: 30

Subject No.: CH31203

Duration: 2 hr

Department: Chemical Engineering

Specific charts, graph paper, log book etc., required: No

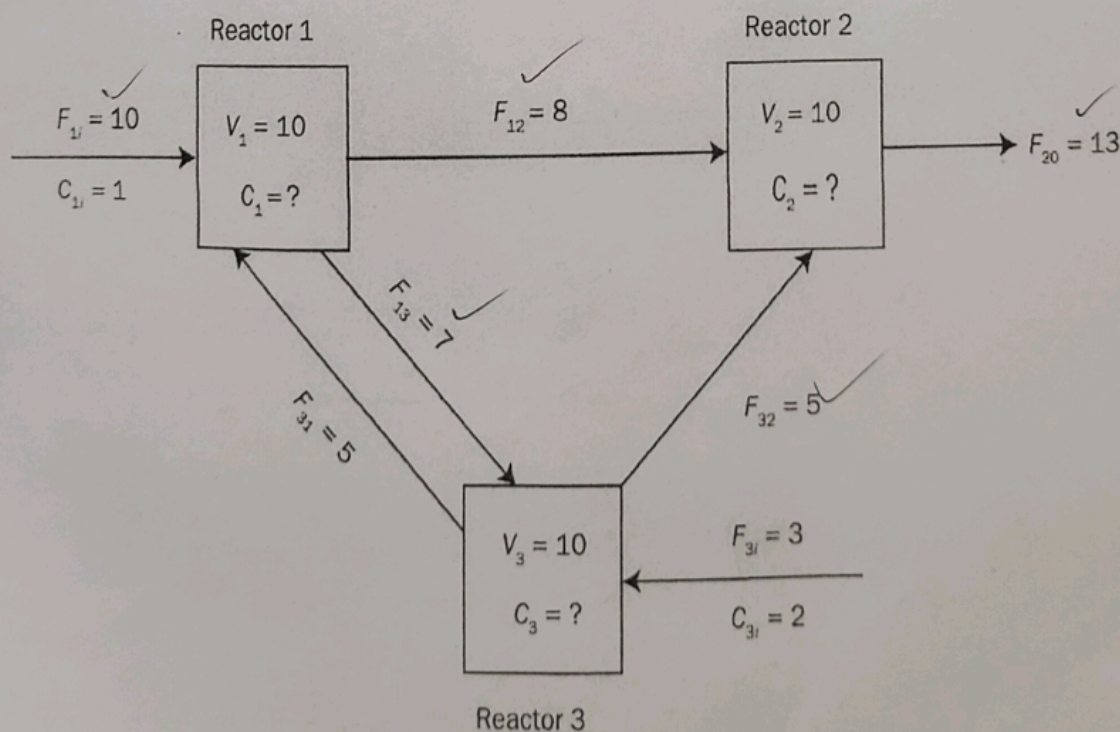
Instructions:

1. Attempt all questions
2. Assume, if necessary, clearly stating the reason
3. Answer all parts of a question together

A system of 3 chemical reactors is shown in Figure 1. In all 3 reactors, a first-order liquid phase chemical reaction,  $A \rightarrow P$ , takes place. The rate of disappearance of reactant  $A$  is given as:  $(-r) = kC$ . Here, the reaction rate constant,  $k = 0.1 \text{ sec}^{-1}$ .

(i) Derive the component  $A$  balance equations for all 3 reactors operated at steady state [5]

(ii) Find 3 concentrations of component  $A$  ( $C_1$ ,  $C_2$  and  $C_3$ ) using the method of Gauss elimination with backward sweep [5]



**Figure 1.** A system of 3 reactors [ $F$  = volumetric flow rate ( $\text{m}^3/\text{sec}$ ),  $C$  = concentration of reactant  $A$  ( $\text{kg}/\text{m}^3$ ),  $V$  = volume of liquid in the reactor ( $\text{m}^3$ )].

2. Find  $x$  at which the following function yields its minimum value:

$$f(x) = x + 2 \sin x$$

[8]

Use N-R method with  $x_0 = -2$  and desired tolerance  $= 10^{-5}$ .

3. (a) Discuss the relative merits and demerits of explicit and implicit Euler.

(b) Consider the following IVP:

$$\frac{dy}{dx} = x + y$$

$$y(0) = 1$$

[2+4+6=12]

Compute  $y(0.5)$  with step size  $h = 0.1$  using the following methods:

(i) RK2

(ii) RK4

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