INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

End-Spring Semester 2016-2017

Subject Name: Computer Methods in Chemical Engineering — Full Marks: 50

Subject No.: CH42006 — Time: 3 hours

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

1. (a) Consider an adiabatic flasher shown in Fig. 1. For this pressure reducing device, the following known and unknown terms are defined: **[5+4+(4+3)+(6+4)+(5+3)=34]**

Known terms: T, L_F, Z_{Fi}

Unknown terms: F, P, x_{Fi}, V_F, y_{Fi}

Develop a computer-assisted simulation algorithm detailing all sequential steps.

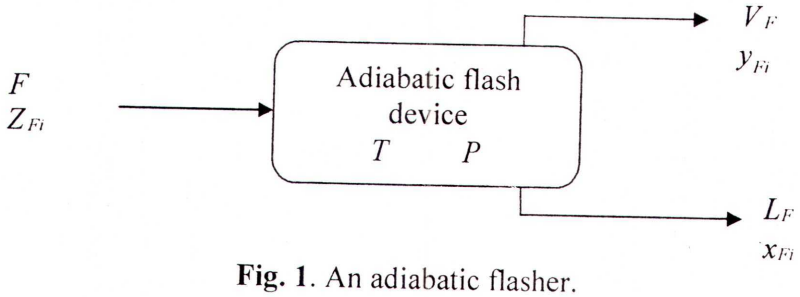

Fig. 1. An adiabatic flasher.

(b) Develop a dynamic model for the U-tube manometer shown in Fig. 2 by performing the momentum balance. As shown, the tube is partially filled with a liquid, and each end of two arms is connected to a pressure (P) source.

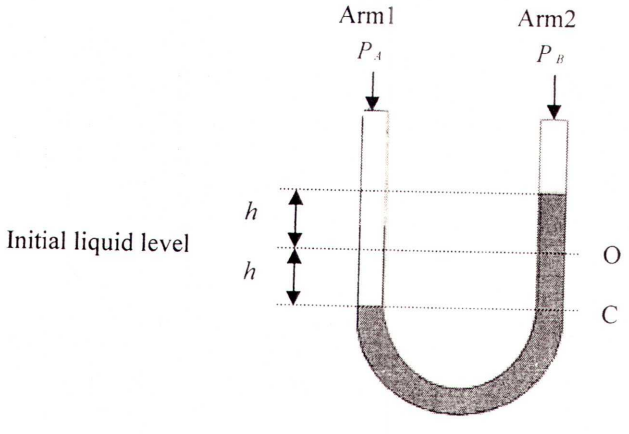

Fig 2. A U-tube manometer.

(c) What are the uses of simulated process model? Discuss the state variable – output variable map with a suitable example.

(d) Considering a first-order irreversible chemical reaction $A \xrightarrow{k} B$, develop an isothermal CSTR model and show its simulation steps with the application of the second-order Runge-Kutta (RK2) method. Represent this model in dimensionless form assuming constant reactor volume.

(e) Develop a rigorous model for a continuous-flow distillation column stating all assumptions. Formulate a computer-assisted simulation algorithm providing all sequential steps.

2. (a) The distribution coefficient (k_D) is given below as a function of phase compositions (x_i^R and x_i^E), temperature (T) and pressure (P): **[(4+4)+(4+4)=16]**

$$k_{Di} = \frac{\gamma_i^R}{\gamma_i^E} = f\left(x_i^R, x_i^E, T, P\right)$$

where, γ denotes the activity coefficient. Deriving the model with suitable assumptions, develop a computer-assisted simulation algorithm with a variable k_D for a liquid-liquid extractor.

(b) Develop a vaporizer model (stating suitable assumptions) and its simulation algorithm.

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