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## COLLEGE OF ENGINEERING

### DEPARTMENT OF CHEMICAL AND PETROLEUM ENGINEERING B.ENG. CHEMICAL ENGINEERING PROGRAMME

#### Computer Applications in Chemical Engineering II (CHE 471) Assignment I

*Given Date: 20/09/2018*

*Submission Period: 12 noon on 25/09/2018*

#### PROBLEM STATEMENT

The information obtained from the literature has shown that model equations for the purities of methanol and butyl acetate obtained from the transesterification reaction occurring between butanol and methyl acetate in a reactive distillation column have been developed to be as given in Equations (1) and (2),

$$\begin{aligned} x_{MeOH} = & -0.738 + 0.058A + 0.0864B + 0.1025C - 2.229D - 0.12223A^2 - 0.00166B^2 + \dots \\ & \dots - 0.003316C^2 - 0.224D^2 + 0.01182AC + 0.4285AD + 0.01941BD + \dots \\ & \dots + 0.02449CD \end{aligned} \quad (1)$$

$$\begin{aligned} x_{BtAc} = & 1.481 - 0.4A - 0.0739B + 0.0414C + 1.681D - 0.0616A^2 - 0.003078C^2 + \dots \\ & \dots + 0.00987AB + 0.01445AC + 0.002063BC - 0.03058BD \end{aligned} \quad (2)$$

where  $x_{MeOH}$ ,  $x_{BtAc}$ ,  $A$ ,  $B$ ,  $C$ , and  $D$  are methanol mole fraction, butyl acetate mole fraction, reflux ratio of the column, butanol volumetric flow rate, methyl acetate volumetric flow rate and reboiler duty, respectively. Using the initial values of the input variables given in Table 1, estimate the values of the parameters required for the maximization of the process variables by carrying out multiobjective optimization using the *fsolve* command of MATLAB. Write the maximum values obtained for the process variables.

Table 1. Initial values of the input variables

Parameter	Value
Reflux ratio	3
Butanol flow rate (mL/min)	25
Methyl acetate flow rate (mL/min)	10
Reboiler duty (kJ/s)	0.7

**Hint:** It is not mandatory to get exactly one (1) as the maximum mole fraction of a product from a process, even if the target is 1.