UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

B.Eng. *M.Eng.*

Chemical Eng E862: Computer Aided Process Engineering

COURSE CODE	:	**CENGE862**
UNIT VALUE	:	**0.50**
DATE	:	**25-MAY-05**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours**

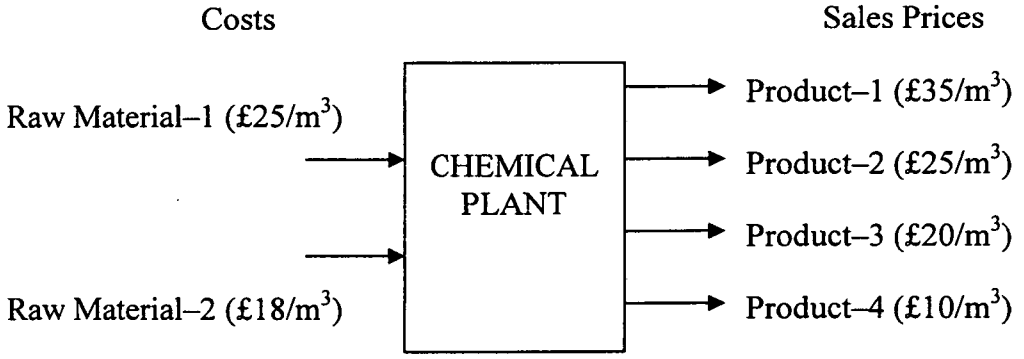
05-C0189-3-60

TURN OVER

*Answer **THREE** questions.* **Only the first THREE answers will be marked.**
*ALL questions carry a total of **20 MARKS** each, distributed as shown* [ ]

1.

The figure shows the schematic of a chemical plant that processes two raw materials to produce four products, where cost and selling prices are given in the parentheses.



The yields of the two raw materials and the maximum allowable production of the products are given in the following table.

	Volume Percent Yield		Maximum Allowable Production (m^3/day)
	Raw Material–1	Raw Material–2	
Product–1	75	45	24000
Product–2	3	7	1500
Product–3	12	35	5000
Product–4	10	13	unlimited

Processing cost of raw material–1 is £0.75/m^3 and that of raw material–2 is £1.00/m^3. The objective is to maximize profit where the profit is given by:

Profit (£/day) = Income by selling the products – raw material costs – processing cost.

Let x_1 (m^3/day) and x_2 (m^3/day) denote the amounts of the raw materials–1 and 2, respectively, that must be purchased.

(a) Formulate the problem as a linear program in terms of x_1 and x_2. [8]

(b) Calculate x_1 and x_2 that maximizes the profit by using:

i. The graphical method, [6]
ii. The Simplex method with $x_1 = x_2 = 0$ as the initial basic solution. [6]

PLEASE TURN OVER

2.

i) In the equation based formulation of flowsheeting problems why is it necessary to reduce the occurrence matrix to a square matrix? What must be done to make the occurrence matrix square? [4]

ii) What is meant by a torn stream? [2]

iii) Give simple equations for the flowsheet in Fig 1. There are five components in the plant (reactant A, by-product I, product B, H_2 and CO_2), two chemical reactions in the reactor, and two separators removing by-product, product and some of the hydrogen and solvent (CO_2). Each separator may be modelled with a component separator. How many degrees of freedom are there in the problem? [6]

iv) What is the difference between a simulation problem and a design problem? Give an example of each for the problem in part iii). [4]

v) A binary dew point calculation can be solved without iteration. Show the formulation of the problem. [4]

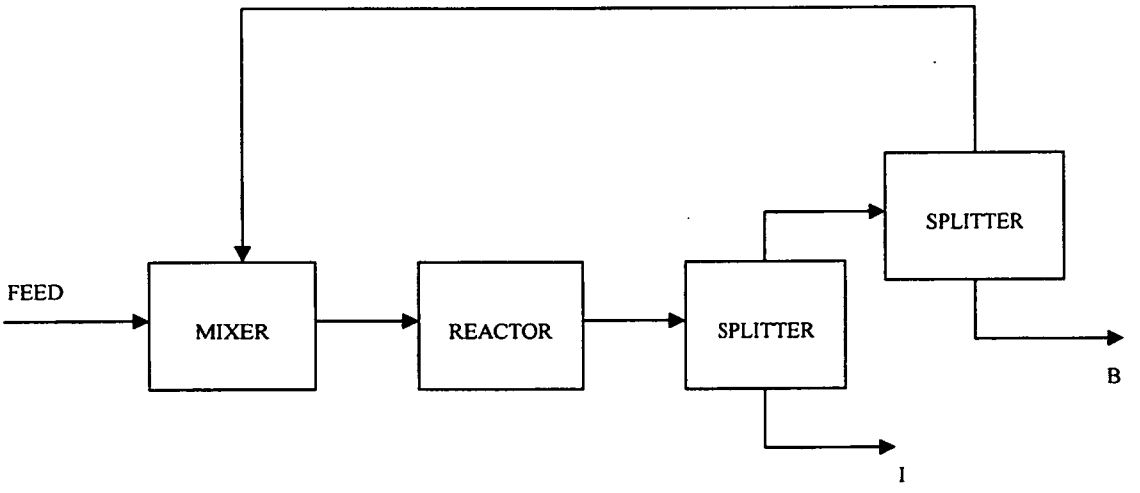


Figure. 1

PLEASE TURN OVER

3.

i) What is the formula which generates the Newton step, **p**, for a set of nonlinear algebraic equations, **f(x)** = **0**. Define all your terms. [4]

ii) What is meant by a difference approximation for a Jacobian matrix of a set of equations? [3]

iii) What is meant by the Constant Matrix method for solving a set of nonlinear algebraic equations. [3]

iv) Obtain the new iterate **x** using Newton's method for the following problem starting from the point $\mathbf{x}^T = [2 \;\; 1]$

$$f_1 = x_1^3 + x_1 x_2 - 3$$
$$f_2 = x_1 + x_2^3 - 5$$

[6]

v) What is meant by an ill conditioned set of equations? Why does this cause problems for Newton type methods? [4]

4.

(a) The Leibniz formula tells us that

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \ldots$$

We can use this formula to calculate the value of π to as many digits as we would like. Write the Matlab code to determine how many terms of the above expressions we need to get a value of 3.1415. Include all appropriate error checking. Comments in the program are not necessary. Describe how your program works. [12]

(b) Give two reasons for using functions in Matlab. [2]

(c) The following code is part of a larger program which implements the Simplex method. This code fragment is responsible for doing the Gauss-Jordan elimination step. Improve this code by adding any necessary error checks.

```
function A = GJ(A, row, column)
 [m n] = size(A);
 for i = 1:m
  if i ~= row
A(i, 1:n) = A(i, 1:n) - A(row, 1:n) * A(i,column)/A(row,column)
  end
end
 A(row, 1:n) = A(row, 1:n)/A(row,column)
end
```

[6]

PLEASE TURN OVER

5.

(a) Define mathematically a first order initial value problem and a second order boundary value problem. [4]

(b) Derive the implicit Euler method for solving initial value problems. Explain the derivation through the use of a diagram. [8]

(c) The following is a second order Runge-Kutta method:

$$k_1 = \delta t \times f(t_i, y_i)$$
$$k_2 = \delta t \times f\left(t_i + \frac{3}{2}\delta t,\ y_i + \frac{3}{2}k_1\right)$$
$$y_{i+1} = y_i + \frac{2}{3}k_1 + \frac{1}{3}k_2$$

Apply this method once to the initial value problem

$$\frac{d}{dt}y(t) = 1 - y(t)$$
$$y(0) = 0$$

using a time step of $\delta t = 2$. [8]

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