UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualification:-

B.Eng.

Chemical Eng E862: Computer Aided Process Engineering

COURSE CODE	:	**CENGE862**
UNIT VALUE	:	**0.50**
DATE	:	**20-MAY-03**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours**

03-C0193-3-30

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 steady state temperature of a rod of length L, which is heated at one end to a temperature of 400 K and is cooled at the other end to 315 K, can be described by the following boundary value problem:

$$\frac{d^2}{dx^2}T(x) = 0$$
$$x \in [0, L]$$
$$T(0) = 400$$
$$T(L) = 315$$

a) Describe, in detail, how to find an approximation to the temperature profile numerically for $x \in [0,L]$. [8]

b) Write the Matlab code for the solution procedure for general values of L and N, where N is the number of points to use in the discretization procedure. [10]

c) How does the answer for part a) change if the model is changed to

$$\frac{d^2}{dx^2}T(x) = g(x)$$
$$x \in [0, L]$$
$$T(0) = 400$$
$$T(L) = 315$$

for some function g(x)? [2]

2. a) Derive Euler's method for the ordinary differential equation

$$\frac{d}{dx}y(x) = f(x, y(x))$$

using Taylor's series. Recall that the Taylor series expansion of $f(x+\delta x)$ is given by

$$f(x+\delta x) = f(x) + \delta x \times f'(x) + \frac{\delta x^2}{2!} \times f''(x) + \cdots$$

Show the error term due to the Euler approximation. [6]

CONTINUED

b) Apply Euler's method twice, using a step size of 1, to find an approximation to y(2) for the following initial value problem:

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

[4]

c) The improved Euler method consists of two steps:

$$y^* = y(t) + \delta t \times f(t, y(t))$$
$$m^* = f(t + \delta t, y^*)$$
$$y(t + \delta t) = y(t) + \delta t \times \frac{f(t, y(t)) + m^*}{2}$$

Write a Matlab procedure which implements this method. You may assume that a function `f(t,y)`, initial value `y0` and step size `dt` have been provided. The stopping criterion will be to find the solution at time `tfinal`.
[10]

3. As an Engineer you have professional responsibilities in the use of computers in everyday work, in particular in ensuring that the program is 'fit for purpose'. The following process to guide you was presented.

define your problem
select the program
prepare and check the input
solve the equations (ie. run the program)
check the results
keep proper records

What are the three key aspects you should ensure for the first stage 'define your problem'? [3]

a) What is meant by the degrees of freedom of a flowsheet? [2]

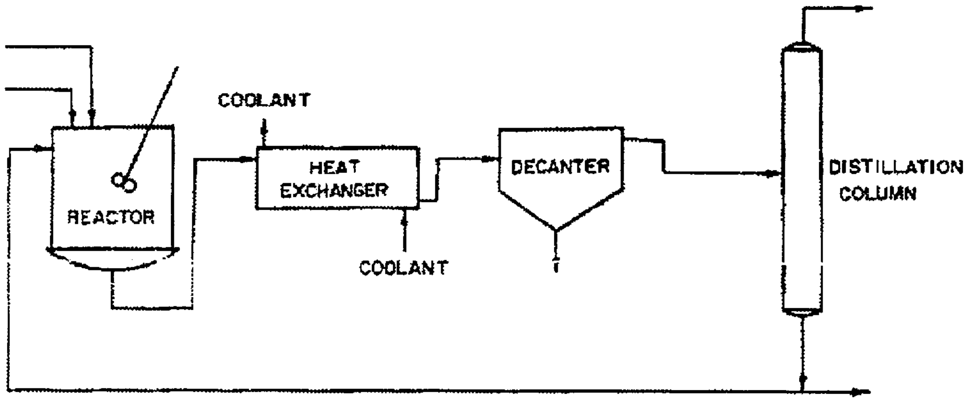
b) How can the number of degrees of freedom of a flowsheet help in determining the specification required to solve a design problem? [3]

c) What is meant by the occurrence matrix of a flowsheeting problem? [3]

d) In what way can the occurrence matrix be used to determine the number of degrees of freedom? [3]

CONTINUED

e) Set out the equations and variables for the problem in the diagram below and determine the number of degrees of freedom. Assume that only one reaction takes place in the reactor and consider the mass balance only. [6]



4. a) Define the Jacobian matrix, J, of a set of algebraic equations **f(x)**. [3]

b) Show why the standard Newton algorithm would fail to solve the following problem if the initial point used to start the algorithm was $x_1 = 0$ and $x_2 = 0$

$$2x_1x_2 + 3x_2 - 1 = 0$$
$$x_1^2x_2 - 1 = 0$$ [5]

c) Suggest another initial point that would also cause the algorithm to fail for the same reason. [2]

d) Obtain the new iterate **x** using Newton's method for this problem starting from the point $\mathbf{x}^T = [2 \;\; 1]$ [5]

e) Show graphically whether the algorithm is converging to the solution. [5]

5. a) Find with the aid of a graph, the solution to the following optimisation problem:

Maximise $f(\mathbf{x}) = 2\,x_1 + x_2$

Subject to: $-x_1 + x_2 \leq 1$ (A)

$x_1 \leq 4$ (B)

$x_1, x_2 \geq 0$

Identify the feasible region on the graph as well as the optimum if one exists. [4]

b) What is the new optimal solution if constraint B is removed? [2]

CONTINUED

c) The Simplex method with Gauss-Jordan elimination is to be used to find the optimal values of x_1 and x_2 as well as that of $f(\mathbf{x})$. Construct an initial Simplex tableau for the problem described above. [4]

d) Find the optimal values of x_1 and x_2 as well as that of $f(\mathbf{x})$, using the Simplex method with Gauss-Jordan elimination starting from the initial tableau constructed above. Use the origin as your initial basic solution. Identify the basic and non-basic columns at each step. Indicate clearly on your graph from a) the points to which *each* Simplex tableau corresponds. [8]

e) Explain briefly what a Mixed Integer Programming problem is and give three chemical engineering examples of such problems. [2]

END OF PAPER