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	:	**13-MAY-04**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours**

04-C0192-3-60

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.

a) Explain in terms of the digital representation of numbers why computer operations have a limited accuracy. [3]

b) What are roundoff errors? [4]

c) You have responsibility for the decisions you make using computational tools. In order to ensure that the tool is 'fit for purpose' you must clearly define your problem. What three points were recommended to define your problem? [3]

d) A process to produce a specialty chemical involves the following hydrogenation reaction $A + H_2 \rightarrow B$ in the presence of a solvent S, followed by a flash separator. The flash separation separates some of the H_2 and the solvent into the liquid stream which is fed back to the reactor after addition of the feed stream of A and solvent and H_2 makeup. All the product is removed in the vapour stream. The company wishes to set up a simple recycle calculation and including the temperature dependence of the flash separation on a spreadsheet to undertake sensitivity studies. You may assume that the vapour liquid equilibrium relations are given. Set up the equations that would be necessary to solve the problem and determine the number of degrees of freedom. [8]

e) It is necessary to determine the feed stream and make up stream conditions given a fixed pressure for the system described in part d). Suggest a sensible set of specifications which would allow you to solve the problem. [2]

2.

The following is a general form of the Newton algorithm for solving sets of nonlinear equations:

1) Guess $\mathbf{x}^0$ and set iteration counter to k = 0
2) Evaluate $\mathbf{f}(\mathbf{x}^k)$
3) Check for convergence
4) Check that the maximum allowable number of iterations has not been exceeded
5) Determine the new guess for $\mathbf{x}^{k+1}$
6) Increment iteration counter, k
7) Return to step 2

a) Give two alternative ways of implementing step 3 and two for step 5 [6]

CONTINUED

2. continued

b) What is meant by an ill-conditioned set of equations? Why might this characteristic cause Newton methods difficulty? What can be done to alleviate the situation? [6]

c) The following set of two equations is to be solved by the Newton algorithm:

$$f_1(x) = 100\,(x_2 - x_1^2)^2$$

$$f_2(x) = (1 - x_1)^2$$

Starting from the point [0, 0] perform one iteration of the algorithm above using the actual Jacobian matrix. [8]

3.

a) Define, briefly, what is meant by objective function, equality and inequality constraints and feasible region. [3]

b) Find, with the aid of a graph, the optimal solution to the following optimisation problem:

$$\text{Maximise } f(x) = x_1 + x_2$$

subject to

$$x_1 - x_2 \leq 4$$

$$x_2 \leq 6$$

$$x_1, x_2 \geq 0$$

[4]

c) A paint plant produces white and coloured paint. White paint is produced in two reactors, W1 and W2, and coloured paint is produced in one reactor, C1. Reactor W1 has a fixed capacity of 4 units per day. The production of white paint in W2 depends on the production of coloured paint, i.e. the amount of white paint produced in W2 is less than or equal to the amount of coloured paint produced in reactor C1. There is no capacity constraint on reactor W2. Coloured paint is only produced in reactor C1 which has a maximum capacity of 6 units per day. The net profit is £1 per unit for both white and coloured paints.

Construct the initial Simplex tableau for this problem when the objective is to maximise the daily net profit. Define the initial basic and nonbasic variables. What is the significance of specifying these values? [5]

d) Find the optimal daily profit and the production of white and coloured paints using the Simplex method. [8]

PLEASE TURN OVER

4.

a) In the analysis of the design of a reactor, you have come across the need to evaluate the following integral:

$$\int_a^b \frac{(1+x)^{o-1}}{(1-x)^o}dx$$

This integral relates the conversion x to the residence time. Although this integral can be evaluated numerically for some values of o, a numerical approach is required in general.

A numerical approach for evaluating an integral is the trapezium rule which is defined as:

$$\int_a^b f(x)dx \approx \frac{\delta x}{2}\left(f(a)+f(b)+2\times\sum_{i=1}^{n-1} f(x_i)\right)$$

where the interval $[a, b]$ has been divided into n sub-intervals of length δx so that $x_1 = a + \delta x$, $x_2 = a + 2\delta x$, ..., $x_n = b$.

Write a Matlab function to implement this numerical procedure. The function must take three arguments, a, b, and n, and return one value, the approximation to the integral. You can assume that a function $f(x)$ has already been defined. Include any appropriate error checking. [10]

b) Give two reasons for writing functions when implementing a program in Matlab. [2]

c) Explain, in detail, what the following Matlab function does:

```
% Given: matrix A, row r and column c indices
  function A = f(A, r, c)
   [m n] = size(A);
   for i = 1:m
     if i ~= r
      A(i, 1:n) = A(i, 1:n) - A(r, 1:n) * A(i,c)/A(r,c)
     end
    end
    A(r, 1:n) = A(r, 1:n)/A(r,c)
  end
```

[6]

d) In the code presented in part (c), what error checking would you add to make the code more robust? [2]

PLEASE TURN OVER

5.

a) Describe, in detail, Euler's method for solving initial value problems. What is the meaning of local truncation error? What is the local truncation error for Euler's method? [6]

b) Describe briefly how a second order initial value problem can be solved using, for instance, Euler's method. [2]

c) The numerical solution of this second order boundary value problem,

$$\frac{d^2}{dx^2}y(x) = 0$$

$$y(0) = y_A$$

$$y(1) = y_B$$

can be based on the application of the central differences operator to approximate the second derivative term. What is this central difference operator? The result of this operator is a tri-diagonal system of equations. Write the Matlab code to initialise and solve this system of equations given a number of sub-intervals, N, for the discretization of the spatial domain. [12]

END OF PAPER