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	:	**12-MAY-06**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours**

TURN OVER

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

Graph paper provided

1.

The following is the algorithm for Newton's method for solving sets of nonlinear equations:

(i) Guess x^0 and set iteration counter to k=0
(ii) Evaluate $f(x^k)$
(iii) Check for convergence
(iv) Check that the maximum allowable number of iterations has not been exceeded
(v) Determine the new value for x^{k+1}
(vi) Set k to k+1 and return to step (ii)

a) The effectiveness of particular implementations of Newton's method on particular problems is judged in terms of the reliability and the efficiency of the algorithm. What is meant by these two terms? [2]

b) Give some alternatives for step (v) and discuss the effect on reliability and efficiency of the algorithm. [4]

c) What is the role of Gaussian Elimination in this algorithm? [1]

d) What might cause the Gaussian Elimination procedure to fail and what would you do to try and restart the algorithm to get a solution to the nonlinear equation set? [5]

e) Obtain the new iterate $\boldsymbol{x}$ using the Newton's method for the following problem starting from the point $\boldsymbol{x}^T = [1 \quad 1]$

$$f_1 = x_1 x_2 - x_2^2 - 3 = 0$$
$$f_2 = x_1^3 + 4x_2 + 5 = 0$$

[8]

2.

a) What is meant by the degrees of freedom of a flowsheet? [1]

b) Give the strengths and weaknesses of Sequential Modular and Equations Oriented flowsheeting solution strategies and software. What is a torn stream? [5]

c) Consider the flowsheet given in Figure 1. Give mass balance equations for the flowsheet for the case when there are n components in each stream. How many degrees of freedom are there in the problem? [6]

CONTINUED

d) For the equations obtained in part c), specify some variables and obtain a square occurrence matrix for $n = 3$, i.e., a three component system consisting of A, B and C with elementary reaction A→B taking place in Reactor-1 and B→C taking place in Reactor-2. [8]

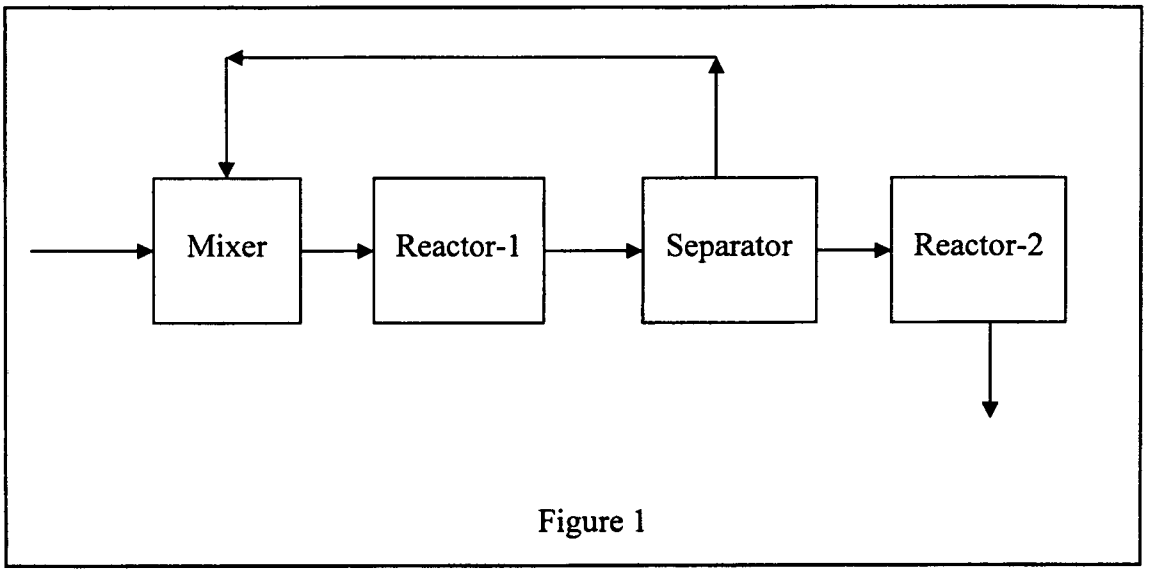

Figure 1

3.

a) Consider the following optimisation problem:

$$\min f(x) = -x_1 - x_2$$

subject to

$$-x_1 + 2x_2 \leq 4$$
$$3x_1 + x_2 \leq 9$$
$$x_1, x_2 \geq 0$$

Compute the optimal solution of this problem by using:

(i) The graphical method, [6]

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

b) What is shadow price? For the problem in part a) which constraint is the optimal value of the objective function most sensitive to and why? [4]

c) What are the advantages of formulating and solving the dual of a linear program? [4]

TURN OVER

4.

a) The fixed point iteration method, also known as repeated substitution, is a method for finding the root of $f(x)=0$ by rearranging this function into the form $g(x)=x$. The method is described by the following recurrence relation:
$x_{k+1} = g(x_k),\ k = 0,\ldots$
which is repeated until the solution x which satisfies $g(x)=x$ is found. An initial guess, x_0, is required to start this procedure.

Write a Matlab program which implements the fixed point iteration method, ensuring that all appropriate error checks are made and appropriate stopping criteria are implemented. Itemize in detail any other information that is required to apply this procedure. [12]

b) Suppose that we wish to find the root of

$$f(x) = x\sin x - 3$$

using the fixed point iteration method. Suggest two alternative g(x) functions which could be used with the fixed point iteration method. Which would you recommend and why? [6]

c) What does the following Matlab code segment do:

```
A = [ 1, 2; 2, 0];
b = [1; 1];
x = A\b;
```

[2]

5.

a) Describe, in detail, the Improved Euler method for solving initial value problems, showing how it is derived. [8]

b) The Euler method is derived by using the forward difference operator to approximate the derivative term in an ordinary differential equation. If the backward difference approximation were used instead, the result would be a method that is known as the Backward Euler method. Derive this method. Why is this method more difficult to apply in general than Euler's method? [4]

c) Apply two steps of the Euler method to the initial value problem:

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

using a time step $\delta t = 1$. [6]

d) Describe the difference between local truncation error and global error when referring to solution methods for initial value problems. [2]

END OF PAPER