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	:	**20-MAY-02**
TIME	:	**14.30**
TIME ALLOWED	:	**2 hours**

02-C0188-3-80

TURN OVER

*Answer **THREE QUESTIONS** only.*
***ALL** questions carry a total of **20 MARKS** each, distributed as shown* [ ]

1. a) 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 (i.e. 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]

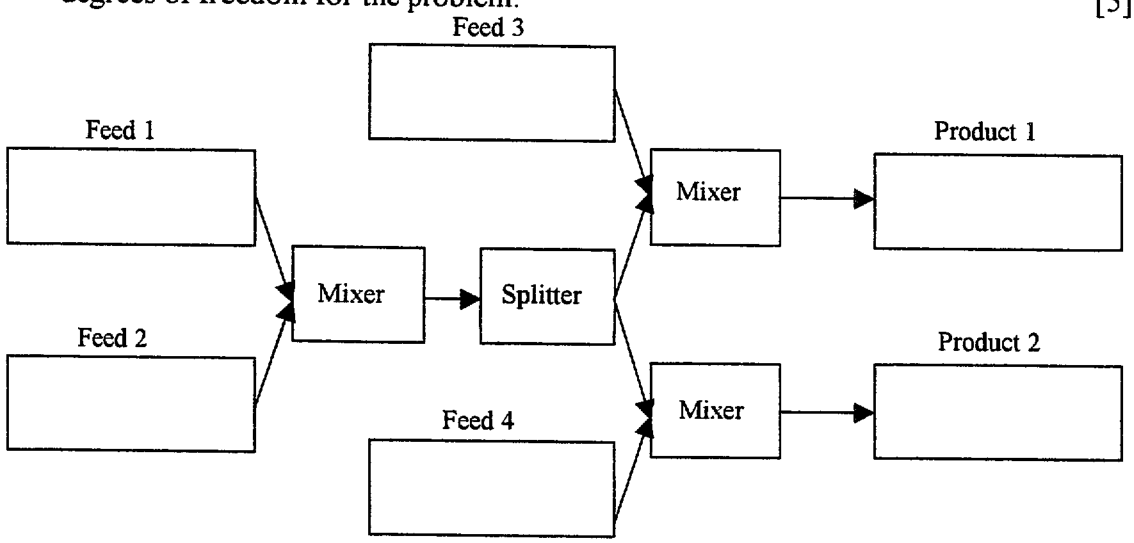
b) What is meant by the degrees of freedom of a flowsheet? [1]

c) Give the strengths and weaknesses of Sequential Modular and Equation Oriented flowsheeting solution strategies and software. [3]

d) Explain how Linear programming is used for developing management scenarios to assist in decision making in the process industries. [4]

e) Why does the Jacobian matrix of a set of equations have the same structural pattern as its occurrence matrix? [2]

f) Set out the equations and variables for the problem in the diagram below, known as a blending or pooling problem, and determine the number of degrees of freedom for the problem. [5]



g) For the problem described in part f), What specifications must be made for the simulation problem and suggest a set of specifications for a potential environmental design problem? [2]

TURN OVER

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

1) Guess $\mathbf{x}^o$ 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) Set k to k+1 and return to step 2

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

b) Give some alternatives for step 5 of the algorithm and discuss the effect on robustness 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 a single nonlinear equation for the liquid flowrate of an isothermal flash for one unit of feed at fixed temperature and pressure. [6]

f) Explain how you would use Newton's method to solve the problem in part e). How else could you solve the problem? [2]

TURN OVER

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

Maximise $f(x) = x_1 + x_2$

Subject to: $x_1 \leq x_2 + 4$ (A)

$x_2 \leq 6$ (B)

$x_1, x_2 \geq 0$

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

b) 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(x). Construct an initial Simplex tableau for the problem described above. [4]

c) Find the optimal values of x_1 and x_2 as well as that of f(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 as well as the point on the graph from a) to which the current solution corresponds. [8]

d) In order to improve the optimal solution, it may be possible to change either constraint A to:

$x_1 \leq x_2 + 5$ (A)

or constraint B to:

$x_2 \leq 7$ (B)

It is not possible to change both constraints. Which constraint would you change? Explain your answer. [2]

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

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:

$x_{k+1} = g(x_k), \quad k = 0,\ldots$

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

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

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