UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualification:-

M.Sc.

M6: Advanced Process Engineering

COURSE CODE	:	**CENG00M6**
DATE	:	**23-MAY-03**
TIME	:	**14.30**
TIME ALLOWED	:	**3 Hours**

03-N0017-3-40

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Answer ***FOUR QUESTIONS, Question 1 and THREE other questions from the rest of the paper.*** **Only the first four answers will be marked.**
ALL questions carry a total of ***25 MARKS*** *each, distributed as shown* [ ]

1.

Given the following extract from a *Jacaranda* input file (the number at the beginning of each line is not part of the input file and is there for reference only):

```
 1 vle.Phase liquidPhase
 2     comps propane butane pentane
 3     x         0.2     0.5     0.3
 4     flow  "1000 *kmol/hr"
 5     phase liquid
 6     base propane "10 *kmol/hr"
 7     base butane  "10 *kmol/hr"
 8     base pentane "10 *kmol/hr"
 9 end
10 vle.Distillation dist
11     RealSet rec 0.99
12 end
13 vle.ProductTank pure
14     Expression spec "$(x>0.99)"
15 end
```

answer the following questions:

(a) Describe the procedure used by Jacaranda for the automated design of process flowsheets. Explain how lines 6-8, 11 and 14 above would affect the operation of this procedure. [15]

(b) Assuming that the distillation unit is the only processing unit defined in the example above and that the aim is to separate the three components in *liquidPhase* into pure component product streams, draw a superstructure representing the search space generated by Jacaranda. [5]

(c) Suppose that line 11 were changed to

```
11      RealSet rec 0.95 0.99
```

with no other changes made to the input file. What effect would this have on the search space? Be as precise as possible. Suggest a solution that could be generated in this case that would not have been possible without this change. [5]

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2.

a) Give three alternative methods for obtaining gradients for derivative based optimisation methods. [3]

b) Explain what is required for initialisation of derivative based methods and how this can affect convergence. [5]

c) Explain what is meant by a non-convex function and give reasons why convergence of Newton type methods is not guaranteed when objective function or constraints are non-convex. [6]

d) What types of nonlinear functions can be made convex, and give an example. [3]

e) What is the test to ensure that a matrix Z is orthogonal to the set of constraint gradients A? [2]

f) What are the properties that the BFGS Quasi-Newton update maintains in the Hessian matrix? [3]

g) The cost of production (C £/barrel) of a chemical is

$C = 50 + 0.1P + 9000/P$

where P is the production rate (in barrels). What production rate would minimise the cost per barrel and what is the cost? [3]

3.

a) What are the Kuhn Tucker conditions for a constrained minimum? Why are they useful for solving optimisation problems? [2]

b) Determine the minimum of the following constrained optimisation problem (where k is strictly positive k>0):

$\min\ (x_1 - 1)^2 + x_2^2$

subject to $\quad x_1 - x_2^2/k \leq 0$

Whether or not the solution is a true minimum is determined by the value of the parameter k. Explain how you would show which range of values of k ensured a minimum. [5]

c) Show diagrammatically why the Generalised Reduced Gradient method often makes steps outside the feasible region. How does the algorithm correct this and return to the feasible region? [4]

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d) What are the main reasons why Newton based methods may not find the global solution to an optimisation problem? [3]

The basic steps of the Successive Quadratic Programming algorithm for solving constrained optimisation problems is as follows

1. Choose an initial feasible point
2. Solve the Quadratic programming problem for the step direction
3. Line search
4. Solve for the Lagrange multipliers
5. Evaluate the gradients. If the point is a Kuhn Tucker point then stop.
6. Update the Hessian approximation using the BFGS update
7. Set k = k+1 and return to step 2.

Answer the following questions about the algorithm:

e) How does the algorithm attempt to ensure that a descent direction is maintained? [2]

f) The method is based on using 'a quadratic approximation to the Lagrangian'. What is meant by this? [2]

g) Suggest two methods for step 3 and explain how they work. [4]

h) Explain the significance of the Lagrange multipliers. [3]

4.

a) Derive a piecewise linear approximation model for a cost function, *C(X)*, by introducing one binary variable for each linear segment. The cost function can be specified by K points $[\gamma_i, C(\gamma_i)]$, *i.e.* K-1 intervals. [12]

b) Assume two sets of constraints in a mathematical model:

$$Set\_1: \ \sum_i A_i X_i \le B$$

$$Set\_2: \ \sum_j C_j Z_j \le D$$

where X and Z are continuous variables; and A_i, C_j, B and D are given parameter vectors.
Formulate the following logical implications by using 0-1 variables as a mixed integer linear set of constraints.

i) *Only one* set of constraints to be active.
ii) *At least one* set of constraints to be active.
iii) *At most one* set of constraints to be active. [13]

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5.

a) Consider the following cost function, C:

$C = 0$ if $X = 0$

$C = A \cdot X + B$ if $L \leq X \leq U$

where X represents the quantity of a product to be manufactured, A is the marginal cost per product unit and B is the manufacturing set-up cost. L and U represent lower and upper production bounds. How can we model the above function mathematically by a mixed integer linear set of constraints by using 0-1 variables in order to alleviate the discontinuity at the origin? [10]

b) The aim is to fit the 'best' straight line (Y=A X + B) to a given set of K experimental data points [X_i, Y_i]. Based on the *deviations* between the experimental value of Y and the value predicted by the above linear relation, formulate the following two cases as linear programming models:

i) Minimise the sum of the absolute value of the deviations.

ii) Minimise the maximum value of the deviations. [15]

END OF PAPER