National Exams May 2004

98 – Chem – B3: Simulation, Modeling and Optimization

3 hours duration

NOTES:

1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the exam paper, a clear statement of any assumptions made.

2. This is a **CLOSED BOOK EXAM.** Only **Casio** or **Sharp** approved calculators are permitted.

3. The exam consists of seven (7) questions. Any five (5) questions constitute a complete exam paper. If more than five questions are answered, the highest five marks will make up the exam grade.

4. Each question is of equal value.

Q1. A chemical plant is to be built outside a certain community. The perimeter of the community can be approximated by a circle, whose radius is taken to be unity. The plant is considered as a point with coordinates (2, 2), if the origin of the coordinate system is the centre of the circle. Find the coordinates and the magnitude of the shortest and longest distance of the plant from the circular perimeter [such information may be important in plant design, taking environmental considerations into account].

Q2. A chemical company is planning to produce Brand A and Brand B fertilizer. The following preliminary data are available to the design engineers.

BASIS: ONE kTONNE	Brand A Fertilizer	Brand B Fertilizer
Capital required, MU	12,000	32,000
Person-days labour required	150	200
Profit upon sale, MU	24,000	30,000
Rate of production: up to 150 ktonne per year		
Total capital available: 3,000,000 MU		
Person-days labour available: 24,000		

MU: arbitrary monetary unit

(a) Determine the amount of Brand A and Brand B fertilizer to be produced annually in order to maximize the annual profit.
(b) Determine the size of the maximum annual profit.
(c) Sketch (plotting is NOT required) the simplex diagram showing the pertinent vertices, and indicate the feasible set and the vertex belonging to the maximum annual profit.

Q3. Butyl acetate is produced in a CSTR from acetic acid, under specific conditions [ref.: J. M. Smith, Chemical Engineering Kinetics, 3rd edn., Example 4-1,p.132, McGraw Hill 1981] with a rate constant of k = 17.4 mL/mol.min at 100 ^{0}C. The inflow rate is Q = 10 L/min, the active volume is V = 500 L, and the inlet acetic acid concentration is c_i = 0.1 mol/L. The mole balance may be expressed as

$$V\frac{dc}{dt} = Qc_i - Qc - kVc^2$$

Here, “c” is the acetic acid concentration and “t” is time. The reactor is run under steady state conditions, then at some time, the inlet acid concentration suddenly increases to 0.15 mol/L and stays at that value.

(a) Construct an approximate linear mole balance and obtain the closed – form c(t) solution.
(b) Obtain the approximate value of the new steady – state acid concentration from part (a).

(c) Obtain the rigorous value of the new steady – state concentration and compare it to the value in part (b). What does this comparison indicate about the goodness of the linear approximation?

Q4. A fibre – optics device used in a testing laboratory employed by a chemical plant is studied to establish the relationship between the linewidth x (in μm units), and the interconnect delay Y (in ps units), assuming the regression

$$Y = \beta_0 + \beta_1 z + \beta_2 z^2; z \equiv \frac{1}{x}$$

On the basis of seven observations the sample regression parameters $b_0 = 1.58397$; $b_1 = -0.12794$ and $b_2 = 0.39995$ with error variance of 0.23297 have been obtained. Also, $R^2 \approx 1$ was computed. The elements of the C – matrix [$\mathbf{C} \equiv (\mathbf{Z}^T\mathbf{Z})^{-1}$] are as follows: $C_{11} = 2.1406$; $C_{12} = -0.8768$; $C_{13} = 0.07033$; $C_{21} = -0.8768$; $C_{22} = 0.4108$; $C_{23} = -0.03483$; $C_{31} = 0.07033$; $C_{32} = -0.03483$; $C_{33} = 0.003081$.

(a) Test the hypothesis that $\beta_1 = 0$ versus the hypothesis that $\beta_1 \neq 0$
(b) Test the hypothesis that $\beta_2 = 0$ versus the hypothesis that $\beta_2 \neq 0$
(c) Given the values of the critical T – statistic below, what can you infer about the P –values in parts (a) and (b)?
(d) Does the $R^2 \approx 1$ value imply that $\beta_i \approx b_i$; $i = 0,1,2$?

α, Level of significance	0.2	0.1	0.05	0.01	0.001
$t_{\alpha/2}$	1.533	2.132	2.776	4.604	8.610

Q5. The unsteady – state fractional temperature difference distribution Y, in a 15% Cr – 10% Ni rod may be expressed in terms of the error function as

$$Y = erf(\frac{x}{2\sqrt{\alpha t}}); erf(u) \equiv \frac{2}{\sqrt{\pi}} \int_0^u \exp(-z^2) dz$$

Here, "x" is the distance measured from the warmer end, "t" is time, and the thermal diffusivity is $\alpha = 5.27 \times 10^{-6}$ m^2/s. It is known that at x = 50 cm and t = 3.294 h, Y = erf(1) = 0.8427.

(a) Estimate Y at x = 60 cm at the same time, by using a first order approximation.

(b) Estimate Y at x = 60 cm at the same time, by using a second order approximation.
(c) Compare the estimates in parts (a) and (b) with the true value of 0.9108.

Q6. A polluted aquifer is treated biochemically. At the outset, and one year later y, the dimensionless pollutant concentration is 1. The variation of y with time is believed to follow the discrete model

$$y_{n+2} - y_{n+1} + \frac{12}{49} y_n = 0$$

(a) Obtain a closed – form relationship for y_n versus n. Hint: The finite difference operator E, defined as $E(y_n) = y_{n+1}$, can be advantageously used. This operator has the same algebraic properties as its "cousin", the differential operator $D \equiv d/dt$ (t is time).

(b) What fractional pollutant concentration can you expect, according to this model 10 years after treatment has started? Assume that the aquifer is not exposed to pollutant after treatment.

(c) Would the aquifer be eventually pollutant – free, if it were not exposed to pollutant after treatment?

Q7. Circle the letter pertaining to what you consider to be the right answer to the following statements.

1. The usefulness of the Kuhn – Tucker theorem in the classical theory of constrained optimization is limited by (a) the dimensionality of the objective function; (b) the position of the optima in space; (c) the numerical difficulty of locating a saddle point; (d) the number of constraints.

2. The Fibonacci numbers used in univariate search for optima are defined as (a) $F_0 = F_1 = 1$; $F_n = F_{n-2} + F_{n-3}$; $n \geq 3$; (b) $F_0 = 0$; $F_1 = 1$; $F_n = F_{n-1} + F_{n-2}$; $n \geq 2$; (c) $F_0 = 1$; $F_1 = 2$; $F_n = F_{n-1} + F_{n-2}$; $n \geq 2$; (d) $F_0 = F_1 = 1$; $F_n = F_{n-1} + F_{n-2}$; $n \geq 2$.

3. In a simplex method, the objective function is evaluated at (n+1) mutually equidistant points in the space of the n independent variables, and these points form the vertices of a regular simplex. This method was devised by (a) Powell; (b) Bellman; (c) Spendley, Hext and Himsworth; (d) Rosenbrock.

4. Davidon's linear search technique is one of the (a) gradient methods; (b) univariate search methods; (c) dynamic programming methods; (d) constrained optimization methods.

5. In the "Hemstitching" technique due to Roberts and Lyvers for constrained optimization, (a) search points along a trajectory are "stitched" together by linear line segments; (b) a step is taken in the gradient direction, and a test for constraint violation is made prior to further action; (c) the rank of the inverse matrix of second derivatives is reduced in order to apply linear constraints; (d) quadratic convergence to the true optimal point is guaranteed.

6. The strategies called "exploratory moves", and "pattern moves" are utilized by an optimization method introduced by (a) Davies, Swann and Campey; (b) Nelder and Mead; (c) Campey and Nickols; (d) Hooke and Jeeves.

7. The square – root key on your simple ("four function") calculator suddenly malfunctions and you decide to use Newton's root – finding method to estimate the square root of a real number A. The correct iteration scheme to use is (a) $x_{n+1} = (x_n^2 - A)/3x_n$; (b) $x_{n+1} = (x_n^2 + A)/(x_n + 2)$; (c) $x_{n+1} = (x_n^2 + A)/2x_n$; (d) $x_{n+1} = (x_n^3 + A)/2x_n$.

END OF EXAM