

National Exams May 2002

98 - Chem - B3: Simulation, Modelling 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, but candidates may use (a) one of two calculators, the CASIO approved models, or SHARP approved models, and (b) a scaled (cm or inch) ruler.
3. Any five of the seven questions provided constitute a complete paper. If more than five questions are answered, the exam grade will be made up of the five highest marks.
4. All questions are of equal value.

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Q1. Given the unconstrained two - dimensional objective function

$$f(x,y) = 5x^3$$

Establish the nature of the stationary point and examine the claim that $f(x,y)$ has a minimum at the stationary point.

Q2. Using the Lagrange - parameter concept, determine the largest volume, which an upright (i.e. vertical) cylindrical container of radius R and height H can have, if its surface area is to be 5 m^2 . *The container has no cover.*

Q3. A pharmaceutical firm produces vitamin pills, using ingredients P and Q, whose composition is shown below. The ingredients are mixed with a filler weighing at least 85 gram to make batches with a total mass of 100 gram, that are pressed into pills. Each batch must contain at least 12 units of Vitamin A, at least 12 units of Vitamin C, and at least 10 units of Vitamin D.

Ingredient	Vitamin A; unit/g	Vitamin C; unit/g	Vitamin D; unit/g
P	2	1	5
Q	2	4	1

If the unit cost of ingredient P is \$ 2.00/g and of ingredient Q \$ 3.00/g, how many grams of each ingredient per batch will minimize the production cost?

Q4. The variation of octane number (Y) with mixing proportions (x_i) three different gasoline blends has been analyzed by linear regression techniques, and the proposed model, based on experiments, may be written as

$$Y = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3$$

where β_i ; $i = 0, \dots, 3$ are the true (population) regression parameters. Computation via ANOVA yields the partial results shown in the tabulation below:

Source	Degree of freedom	Sum of squares
Model	3	61.8516
Error		
Total	12	99.1116

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Using critical values of the F – distribution assembled below,

- (i) Complete the ANOVA table and test the null hypothesis that the model is statistically not significant against the alternative hypothesis that the model is significant, at a 95%, and at a 99% degree of confidence;
- (ii) Establish the approximate P - value of the test;
- (iii) Assume that a *different* model would yield $f = 5.01$. Would this model represent the data better than the model tested in this question? Explain your answer.

α	0.1	0.05	0.025	0.01	0.005	0.001
$f_{\alpha}(3; 9)$	2.81	3.86	5.08	6.99	8.72	13.90

α : level of confidence; $f_{\alpha}(3; 9)$: critical value at α with first degree of freedom = 3, and second degree of freedom = 9

Q5. The specific rate constant of the gas phase reaction $\text{H}_2 + \text{I}_2 \rightarrow 2\text{HI}$ has the value of $k = 3.368 \times 10^5 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at a temperature of 1000 kelvin. The numerical value of one of the two Arrhenius parameters is $B = 2.0202 \times 10^4$ kelvin. The reaction is first run at 1000 kelvin with an equal hydrogen and iodine concentration of $0.001 \text{ mol cm}^{-3}$. Then, the temperature is raised to 1010 kelvin and both hydrogen and iodine concentrations are lowered to $0.0009 \text{ mol cm}^{-3}$.

- (a) Estimate the rate of the reaction under the new conditions, by an appropriate linearization of the rate equation, using the data above.
- (b) Compute the true value of the rate of reaction. Is it in good agreement with the result of linearization?

Note: The Arrhenius equation is $k = A \exp(-B/T)$, where A and B are physical constants.

Q6. The growth of a sediment layer (produced by an unwanted side reaction) depositing on the bottom of an autoclave had been monitored, and the following finite difference (discrete) model was consequently proposed:

$$y(n + 2) - 3y(n + 1) + y(n) = 0$$

where $y(n)$ is the layer thickness in coded units at the end of the n - th week; $y(0) = 0$, and $y(1) = 1$.

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- (i) Derive the closed - form relationship between $y(n)$ and n ;
- (ii) It is stipulated that the sediment be removed from the autoclave when the coded layer thickness reaches the value of 1000. How many weeks are expected to lapse, according to the model, before an originally sediment - free autoclave has to be cleaned out?

Q7. The rate of algae growth in an aquifer is modelled by the nonlinear equation

$$dy/dt = \exp(t^{1/2}) - 2t \quad t = 0; y = 0$$

where time "t", and algae concentration "y" are coded quantities.

- (a) Replace the exponential term by an appropriate, analytically integrable approximating function, and obtain via integration an *approximate* value of the coded algae concentration at 0.1 coded time units.
- (b) Compare your answer to the coded value of 0.113807, obtained by a highly accurate numerical integration formula.
- (c) Sketch the *qualitative* $y(t)$ relationship predicted by the model from zero time to extremely large times.