

STUDENT VERSION

CHEMICAL OPTIMIZATION

STATEMENT

A laboratory experiment is going on in the Projects Lab of your company. A colleague, a production chemist, comes to you for advice.

Compound A is heated to 120°C in order to produce compounds B and C. The temperature of the pot containing all of these compounds is kept at 120°C in order to keep the reaction going. k_1 is the reaction rate constant in units 1/hr for the reaction in which A is converted to B while the reaction rate of converting compound B to C is k_2 . The reaction is shown in (1).



The data from the reaction has been gathered and presented in Table 1.

The goal is to produce compound B for marketing. Thus we seek a mathematical model as an aid in telling us the best time to stop the process and extract compound B for the market. One measure of best is most profit or net return. We know that A costs \$0.50 per mole and B sells for \$3.50 per mole. Our production engineer friend has found that for compound C we can expect a return of \$0.25 per mole from the recovered C.

Find the optimal shutoff time for this process in order to optimize the net return on this process.

Opportunities

1. Without using any “sophisticated” modeling techniques offer a plausible approach and suggest a method to solve such a problem. Look at the data!
2. Form a mathematical model. Be sure to state your assumptions - mathematical and chemical. Use this mathematical model to tell your corporate friend just when to shut off the process and just how much profit they can expect on this process.

Ideas for modeling consist of curve fitting, differential (rate) equations, or difference equations.

Time (min)	A (mole)	B (mole)	C(mole)
0	1.00	0.00	0.000
2	0.88	0.12	0.003
6	0.69	0.29	0.030
10	0.53	0.42	0.050
20	0.28	0.56	0.16
30	0.15	0.57	0.28
50	0.043	0.46	0.50
70	0.012	0.33	0.66
90		0.22	0.78
120		0.12	0.88
150		0.06	0.94
200		0.02	0.98

Table 1. Data reported from chemical reaction in which chemical A is converted to B and then converted to C.

Post Solution issues, modifications, and more problems

1. Suppose your colleague comes back to you and says that you NOW have to consider the optimization in view of the energy costs to run the process and it is known that the energy costs to run this process are \$0.005/hr.

Formulate a model which will find the optimal shutoff time for this process in order to optimize the profit on this process.

2. Compare your results when you consider energy to when you do not.
3. Finally attempt to determine the sensitivity of yield and final net return in terms of changes in the energy cost. Namely offer a plot of profit and change in profit/unit change in price of energy (marginal profit) as a function of price of energy, say in the range $[0, 0.04]$, i.e. from no costs to approximately 8 times the current costs of \$0.005/hr.

REFERENCES

- [1] Law of mass action. 2015. *Encyclopdia Britannica Online*. <http://www.britannica.com/science/law-of-mass-action>. Accessed 16 September 2015.