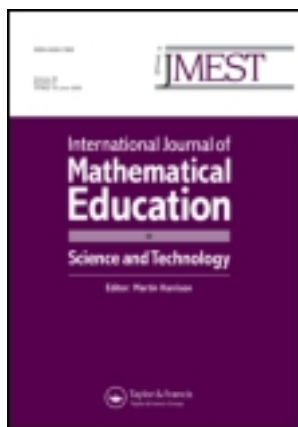


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Parameter estimates in differential equation models for chemical kinetics

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Parameter estimates in differential equation models for chemical kinetics

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(Received 19 February 2010)

We discuss the need for devoting time in differential equations courses to modelling and the completion of the modelling process with efforts to estimate the parameters in the models using data. We estimate the parameters present in several differential equation models of chemical reactions of order n , where $n=0, 1, 2$, and apply more general parameter estimation approaches to an optimization problem involving the production chemical reaction $A \rightarrow B \rightarrow C$.

Keywords: parameter estimation; modelling; differential equations; chemical kinetics; optimization; linearization; sum of square errors

1. Introduction

When teaching differential equations to students we believe it is imperative to motivate the study with rich applications in disciplines that relate to what students are doing in other courses and to the real world beyond academe. Students have difficulty with developing their own conceptual framework of what a differential equation really represents. Indeed, in our teaching over the years (some 40 years) we have found students to disparage the study of differential equations (1) in the abstract and (2) in application. When studying differential equations in the abstract students have a great deal of difficulty in answering their own internal questions, ‘Why do they want us to start with information about a derivative in order to get information about a function? Why not just start with the function itself?’ or ‘Who would ever start with a question when what we want is an answer?’ In application, when given some data and asked to model the situation with a differential equation, students really balk at building a differential equation to get to a relation or function which will model the data. They say to themselves (and the brighter they are, the more confident they seem in this belief and the more they balk), ‘Why not just go right to the function and fit it to the data?’ for many of them have had some modelling experience with data in which they put a least squares line through data or jam an arbitrary degree polynomial through a data set. They just do not see a reason

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for the step that goes first to a differential equation and then to a solution, a function or relation. Nor do students see a need to build a model with meaning in which parameters have units and interpretation and then obtain estimates for these parameters using the data and the differential equation model itself, either analytically or numerically solved.

This effort to estimate parameters is one approach to validate the model itself, for if the model can be fit to the data then that is part of validation and if the estimates and units of the parameters fit our conception of the situation that too is a further validation of our model.

Finally, we do not give our students sufficient practice in parameter estimation in a differential equations course, nor do texts really offer encouragement or space for such activities. However, parameter estimation is one way for completing the act of modelling that gives feedback to the model formulation and solutions. This article is about offering opportunities for parameter estimation. This failure on our part to not discuss parameter estimation in more detail or to provide opportunities to do just that – estimate parameters – would be forgivable if we really had to concentrate on all the methods for solving differential equations we learned as students ourselves. However, in the face of such tools as *Mathematica* and *Maple* where we can get solutions to differential equations, either analytical or numerical, with modest syntax learning and a push of a few keys, it is unforgivable that we do not address the full modelling process in our introductory and advanced differential equations studies.

One way to break students of this belief that they can go directly after a function and not take the circuitous (it looks painful as well) route to a differential equation and *then* a function is to start with a physical phenomenon and build a mathematical model, a differential equation model. If the students have a reasonable amount of physics background in the study of motion then one can appeal to knowledge of Newton's Second Law of Motion and produce a differential equation using $F = m \cdot a = m \cdot x''(t)$ and set it equal to the sum of all the external forces acting on a body, e.g., gravity and media resistance. The same goes for electrical circuit theory as a setting for differential equation modelling. Another way to help students cope with a reasoned and student built differential equation is to appeal to related disciplines of chemistry with attention to rates of reaction or biology with its population rate models of ever increasing complexity. Notice the implied notion of differential equation in the word *rate* in both situations. Often chemistry and biology are easier to motivate than physics and the intrinsic value of the application of differential equations has some spill over into the discipline itself so as to keep students' interest.

In this article, we show two different applications of differential equations, each of which involves building a model, 'solving' these equations, estimating the parameters involved from the data at some stage in the process, and then affirming that our derived function model from the differential equation setting, with the estimated parameters, does a good job of fitting and explaining the data. We do this in two contexts:

- simple chemical reactions and order kinetics from chemistry text books used by the students and
- more complex chemical reaction $A \rightarrow B \rightarrow C$ with parameter estimation and optimization.

2. Simple chemical reaction order

A terrific and credible source for data is the introductory chemistry text book at your school. Many of the students will be using or have used the text and taking material from a text in another department certainly perks students' interest.

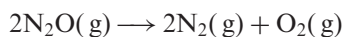
Usually, in each text, there is a section on chemical kinetics with a good number of data sets from documented reactions and lots of mathematical explanations related to the rate (differential) equations which model the reactions. Often the material is motivated by a statement something like, 'The rate of reaction is determined by the concentrations.' This is sometimes referred to as *The Law of Mass Action*. Either through direct collection of data (sometimes easy and sometimes difficult, depending upon the reactants) or referencing a data set from another collection of data one can use this data to model with differential equations. It is known that, 'The rate of decomposition is dependent on the temperature and concentration of the peroxide, as well as the pH and the presence of impurities and stabilizers' [1]. Thus we consider reactions to be dependent upon the concentration of a single reactant, say, A , where $[A]$ is the number of moles of A present at time t . The usual rates of reaction studied in the elementary texts are of the form,

$$\frac{d[A]}{dt} = -k[A]^m, \quad \text{with } [A](0) = [A_0].$$

with k the *rate constant* (presumed to be positive). Usually the study at this level is restricted to $m=0, 1$ and 2 , and these are called *zeroth*-, *first*- and *second*-order reactions, respectively.

2.1. Zeroth-order reaction

Zero-order reactions are most often encountered when a substance, such as a metal surface or an enzyme is required for the reaction to occur. For example, the decomposition reaction of nitrous oxide,



occurs on a hot platinum surface. When the platinum surface is completely covered with N_2O molecules, an increase in the concentration of N_2O has no effect on the rate, since only those N_2O molecules on the surface can react. Under these conditions the rate is a constant because it is controlled by what happens on the platinum surface rather than by the total concentration of N_2O , . . . [2, p. 657].

When considering a generic reaction we shall use $y(t) = [A] = [A(t)]$, the amount of reactant A (often in moles or mol/L) at time t , usually in seconds. Here we see our rate or differential equation is

$$\frac{dy}{dt} = -ky^0 = -k.$$

The solution to this is rather easy, $y(t) = y(0) - kt$. Such reactions are self-evident from the data, for if we plot $y(t)$ versus t we would see a linear function starting at $y = y(0)$ with a negative slope, $-k$. We can easily enter the data in EXCEL and use Trendline to pick off k . Since zeroth-order reactions are quite rare we move on to first-order reactions.

2.2. First-order reaction

Let us look at first-order reactions in general:

$$\frac{dy}{dt} = -ky^1 = -k y \quad \text{with } y(0) = y_0.$$

Using the separation of variables technique we obtain

$$\frac{1}{y} \frac{dy}{dt} = -k,$$

from which we can integrate to see

$$\ln(y) = -k t + c \quad \text{where } c = \ln(y(0)).$$

This gives us

$$\ln(y) = -k t + \ln(y(0)). \quad (1)$$

Now we can actually solve this differential equation for $y = y(t)$ and we do, but the chemist really is interested in determining the nature (order) of the reaction as well as the parameter k , called the *rate constant*, and often stops at this point. Chemists refer to Equation (1) as the *integrated form* of the rate law. They quite often use *this* form of the equation to do their parameter estimation and determination of the order of the reaction. However, in mathematics we might wish to push further to a solution that reads 'y(t) is' – certainly, our function driven students will want to go that far. Thus, after taking anti-logarithms in Equation (1) we can produce a complete solution of our differential equation,

$$y = y(t) = y(0)e^{-kt}$$

but not to our question of order and values for parameters which we address now in several ways.

In the study of chemical reactions, one of the simplest reactions is that of a decomposition of some substance, say hydrogen peroxide (H_2O_2). There is the phenomena of going to the medicine chest to find the hydrogen peroxide (and iodine!) to flush and clean a cut, only to find that what is in the bottle does not produce a white froth when applied to the cut as the medicine is supposed to do while it rids the cut of germs. The medicine is old and has lost its powers! This is an example of decomposition of H_2O_2 into water and oxygen ($2\text{H}_2\text{O}_2 \rightarrow 2\text{H}_2\text{O} + \text{O}_2$) and we use our basic law of mass action to conjecture a rate (differential) equation for $2\text{H}_2\text{O}_2$. This means for $[\text{H}_2\text{O}_2]$ mol/L of hydrogen peroxide:

$$\frac{d[\text{H}_2\text{O}_2]}{dt} = -k \cdot [\text{H}_2\text{O}_2]^m,$$

for some number m . We seek to determine if this reaction is first order, i.e. if $m = 1$.

We return to the task of determining order of the reaction and the parameter k . From Equation (1) we can see that a first-order reaction will produce a linear relationship between $\ln(y)$ and t . In Figure 1(b) we see that there is, indeed, a linear relation between $\ln(y)$ and t . Using EXCEL's Trendline function we find the

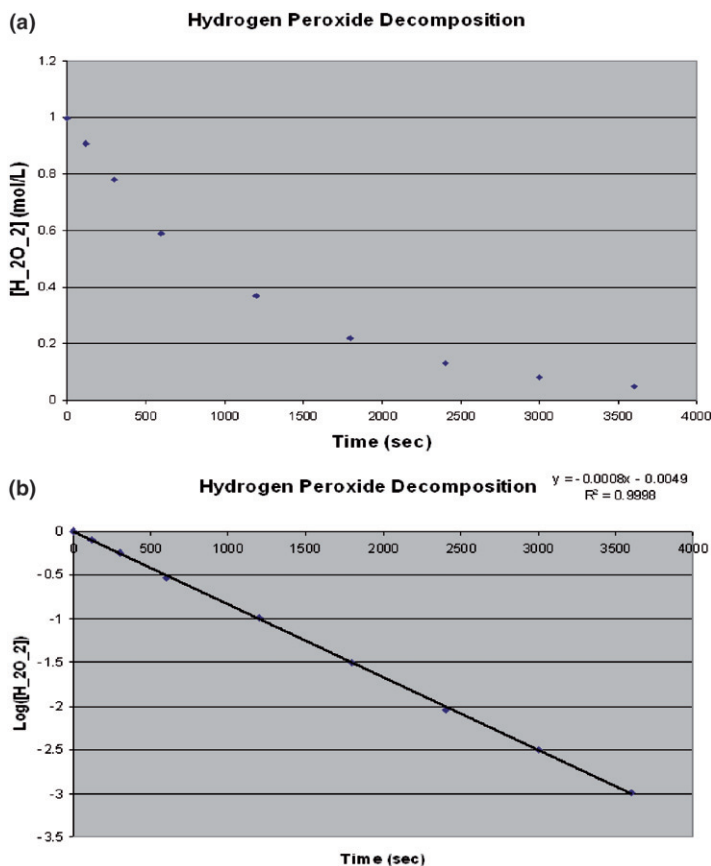


Figure 1. Plots of (a) $[H_2O_2]$ vs. t from Table 2 and (b) $\ln([H_2O_2])$ vs. t from Table 1, the latter showing the linear relationship between $\ln([H_2O_2])$ and t , thus confirming that the decomposition of hydrogen peroxide is a first-order reaction.

following relation

$$\ln(y) = -.0008 t - 0.0049, \quad (2)$$

and from here we can, together with Equation (1), determine that $k = 0.0008$ and so our reaction is first order with parameter $k = 0.0008$.

We can solve Equation (1) with these parameters to produce

$$[H_2O_2] = y(t) = e^{-.0049} e^{-.0008t} = 0.99512e^{-.0008t}.$$

In Table 1, we can see how good our model $[H_2O_2]$ does compared to $[H_2O_2]$ (mol/L). (See Figure 2.) In Table 2 we see the data for Equation (2).

2.3. Second-order reaction

Now let us look at second-order reactions in general:

$$\frac{dy}{dt} = -ky^2 \quad \text{with } y(0) = y_0.$$

Table 1. Collected data and model predicted data on our reaction $2\text{H}_2\text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O} + \text{O}_2(\text{g})$.

| Time (s) | $[\text{H}_2\text{O}_2]$ (mol/L) | Model $[\text{H}_2\text{O}_2]$ |
|----------|----------------------------------|--------------------------------|
| 0 | 1.00 | 0.995111985 |
| 120 | 0.91 | 0.904023431 |
| 300 | 0.78 | 0.782782813 |
| 600 | 0.59 | 0.615758770 |
| 1200 | 0.37 | 0.381021300 |
| 1800 | 0.22 | 0.235769652 |
| 2400 | 0.13 | 0.145890345 |
| 3000 | 0.08 | 0.090274523 |

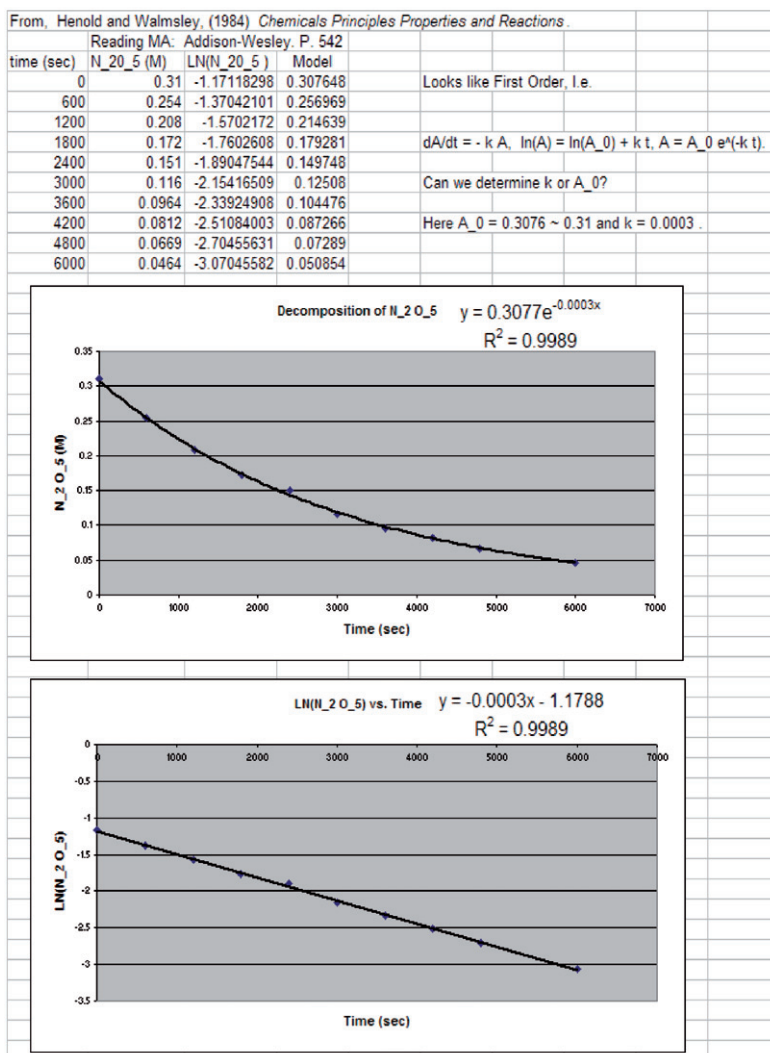


Figure 2. Data for examination of the order of reaction for the decomposition of N_2O_5 [1, p. 542]. Here the reaction is first order.

Source: Ref. [5].

Table 2. Collected data and logged data on our reaction $2\text{H}_2\text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O} + \text{O}_2(\text{g})$.

| Time (s) | $[\text{H}_2\text{O}_2]$ (mol/L) | $\ln([\text{H}_2\text{O}_2])$ |
|----------|----------------------------------|-------------------------------|
| 0 | 1.00 | 0 |
| 120 | 0.91 | -0.040958608 |
| 300 | 0.78 | -0.107905397 |
| 600 | 0.59 | -0.229147988 |
| 1200 | 0.37 | -0.431798276 |
| 1800 | 0.22 | -0.657577319 |
| 2400 | 0.13 | -0.886056648 |
| 3000 | 0.08 | -1.086186148 |
| 3600 | 0.05 | -1.301029996 |

Using the separation of variables technique we obtain

$$\frac{1}{y^2} \frac{dy}{dt} = -k,$$

from which we can integrate to see

$$\frac{1}{y} = kt + c \quad \text{where } c = \frac{1}{y(0)}.$$

This gives us

$$\frac{1}{y} = kt + \frac{1}{y(0)}. \quad (3)$$

Now we can actually solve this differential equation for $y = y(t)$ and we do, but again the chemist really is interested in determining the nature (order) of the reaction and the parameter k and will often stop at this point. For those of us interested in a function for a solution to our rate equation differential equation, after inverting both sides in Equation (3) we have a complete solution of our differential equation, but not our question of order and values for parameters.

$$y = y(t) = \frac{1}{kt + \frac{1}{y(0)}} = \frac{y(0)}{y(0)kt + 1}.$$

In Figure 3 we show a reaction, the decomposition of NO_2 , which is second-order [3, p. 486]. We obtain the rate constant $k = 32.644 (\text{mol/L})^{-1}\text{s}^{-1}$. We confirm the model by computing the predicted model values for $[\text{NO}_2]$ for the observed times. We leave this as an activity for the reader using our estimated parameter value for k .

Let us revisit the decomposition of hydrogen peroxide and show it is *not* a second-order reaction. From Figure 4 we can see that there is no linear relation between $\frac{1}{[\text{H}_2\text{O}_2]}$ and t and hence that the decomposition of $[\text{H}_2\text{O}_2]$ is *not* a second-order reaction.

We reiterate that any first-year chemistry college level text has a myriad of kinetics problems with data and one can motivate the study of differential equations as mathematical models of these order reactions and study the estimations of parameters in the reaction and differential equation with meaning.

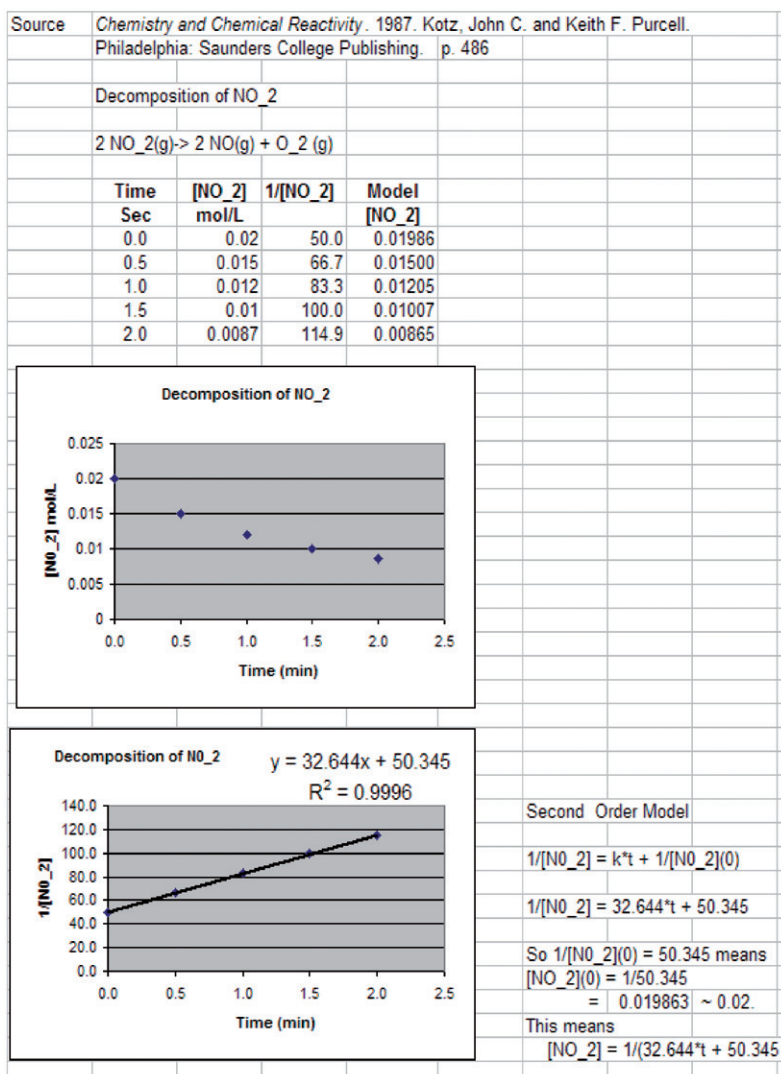


Figure 3. The plot of $\frac{1}{[NO_2]}$ vs. t shows there is a linear relation between $\frac{1}{[NO_2]}$ and t and hence that the decomposition of $[NO_2]$ is a second-order reaction.

Source: Ref. [3].

3. Chemical reaction and optimization

Under a grant from the National Science Foundation¹ a number of complex problems for calculus instruction using technology were offered. These were posted on the web [4]. We discuss one of them here and how it relates to our current discussion of parameter estimation.

The goal here is to make use of kinetics in formulating a mathematical model for a specified chemical reaction, to determine the parameters of the reaction, to confirm the model by comparing its predictions to the data, to formulate the profit function based on the obtained functions for the amounts of the chemicals present at time t

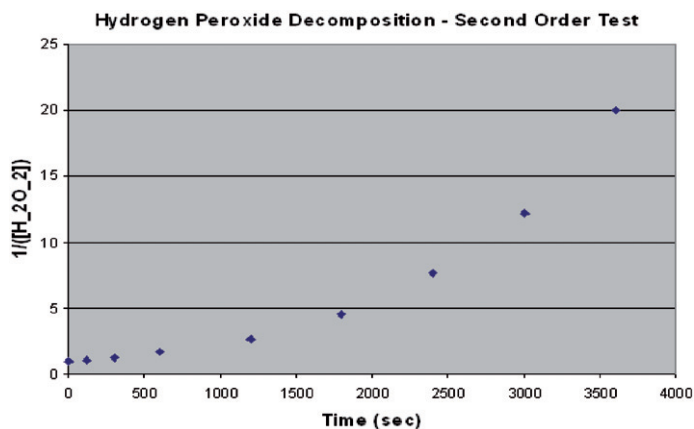


Figure 4. The plot of $\frac{1}{[\text{H}_2\text{O}_2]}$ vs. t shows there is no linear relation between $\frac{1}{[\text{H}_2\text{O}_2]}$ and t and hence that the decomposition of $[\text{H}_2\text{O}_2]$ is *not* a second-order reaction.

Table 3. Collected data on our reaction $A \rightarrow B \rightarrow C$.

| Time (min) | A (mol) | B (mol) | C(mol) |
|------------|---------|---------|--------|
| 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 |

and to optimize profit. Thus, the kinetics and the differential equations are put in the context of a larger applied problem and this makes the problem complex and technology-based. We take a look at the problem in detail.

3.1. Statement of the problem

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.

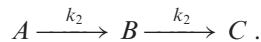
It is believed the reaction is a simple first-order reaction where the reaction rate of converting compound A to B is k_1 1/min and the reaction rate of converting compound B to C is k_2 1/min. The observed data is presented in Table 3.

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. A measure of best is most profit. We are told that A costs \$0.50 per mol and B sells for \$3.50 per mol. Our production engineer friend has found that for compound C we can expect a return of \$0.25 per mol from the recovered C and \$0.05 per mol from the recovered A. You also 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/min. We seek the shutoff time for this process in order to maximize the profit on this process.

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.

3.2. Solution strategies

The first thing students do with data is plot it, obtaining Figure 5. They look at it and see that it makes sense. The reaction starts with only chemical A. B picks up and peaks and the reaction ‘goes to’ C. Using knowledge of first-order kinetics students define variables $a(t)$, the number of moles of A present at time t ; $b(t)$, the number of moles of B present at time t ; and $c(t)$, the number of moles of C present at time t .



They usually build a system of differential equations based on the chemical kinetics of the reaction so they can predict the amount of each chemical present at time t min. From this model they can then run an optimization model in which they seek the time t at which to shut off the reaction in order to optimize their profit.

$$\begin{aligned} a'(t) &= -k_1 a(t), \\ b'(t) &= -k_2 b(t) + k_1 a(t), \\ c'(t) &= k_2 b(t), \end{aligned}$$

We use *Mathematica*'s `DSolve` command to obtain solutions:

$$\begin{aligned} a(t) &= e^{-k_1 t}, \\ b(t) &= -\frac{k_1(e^{-k_1 t} - e^{-k_2 t})}{k_1 - k_2}, \\ c(t) &= \frac{k_1 - e^{-k_2 t}k_1 + (e^{-k_1 t} - 1)k_2}{k_1 - k_2}. \end{aligned}$$

We seek to determine the parameters of the chemical reaction, k_1 and k_2 , that make the solution fit the data best. Thus we enter the data into *Mathematica*. Here is the entering of A's data. We do the same for B and C data.

```
adata = {{0,1}, {2,.88}, {6,.69}, {10,.53}, {20,.28}, {30,.15},
         {50,.043}, {70,.012}, {90,0}, {120,0}, {150,0}, {200,0}}.
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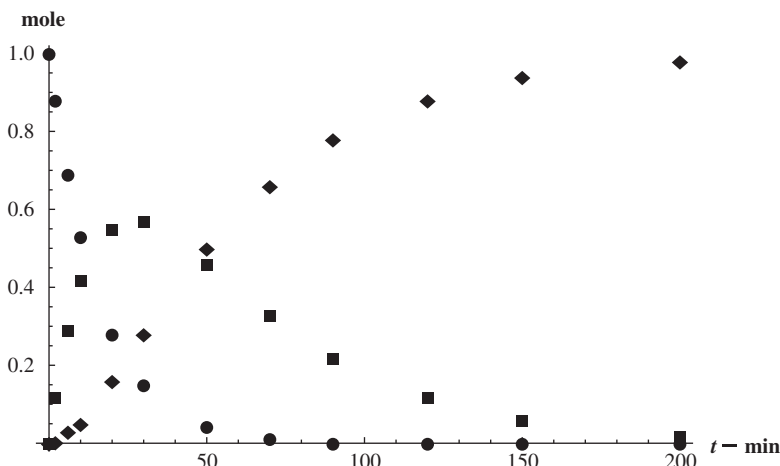


Figure 5. A plot of the amounts of A (●), B (■) and C (◆) as a function of time in minutes. We see the shapes of A declining to zero, B rising and then falling and C rising and levelling off.

From each solution (for $a(t)$, $b(t)$, and $c(t)$) we form a sum of square error terms as a function of the parameters k_1 and k_2 . We show this sum for $a(t)$.

$$SSa[k1_,k2_] = \text{Sum}[(a[\text{adata}[[n,1]]] - \text{adata}[[n,2]])^2, \{n, 1, \text{Length}[\text{adata}]\}].$$

Here $a[\text{adata}[[n,1]]]$ (first number in the n th data point of adata) is actually $a(t_n)$ for the solution at time t_n and $\text{adata}[[n,2]]$ (second number in the n th data point of adata) is the observed amount of A at time t_n . These are then summed over all the observations from $n=1$ to $n=\text{Length}[\text{adata}]$ to form a sum of square error function.

Having formed a sum of square error function for each of the three data sets (we also compute $SSb[k1_,k2_]$ and $SSc[k1_,k2_]$) we then compute a total sum of square error terms using all the data for A, B and C:

$$SS[k1_,k2_] = SSa[k1,k2] + SSb[k1,k2] + SSc[k1,k2].$$

Here is where the power of technology really comes in. We seek to determine the values of our parameters k_1 and k_2 which will minimize $SS[k1,k2]$. The command for this is a one liner:

$$\text{sol}k = \text{FindMinimum}[SS[k1,k2], \{k1, .1\}, \{k2, .2\}],$$

and we can extract the information we want easily with *Mathematica* reporting back,

$$\{1.00038, \{k1 \rightarrow 0.0629595, k2 \rightarrow 0.0211523\}\}.$$

This means the sum of the square errors has a minimum value of 1.0038 when $k_1 = 0.0629595$ and $k_2 = 0.0211523$. If we put these values of k_1 and k_2 back into our differential equation model and solve it with given initial conditions we see the plot of the solution over that of the data in Figure 6.

Of course, since $a(t) + b(t) + c(t) = 1$ we could use only A and B data or only B and C data to obtain our parameter estimates for k_1 and k_2 . Our results are, in fact, slightly different in these cases. For example, if we used only A and B data we obtain

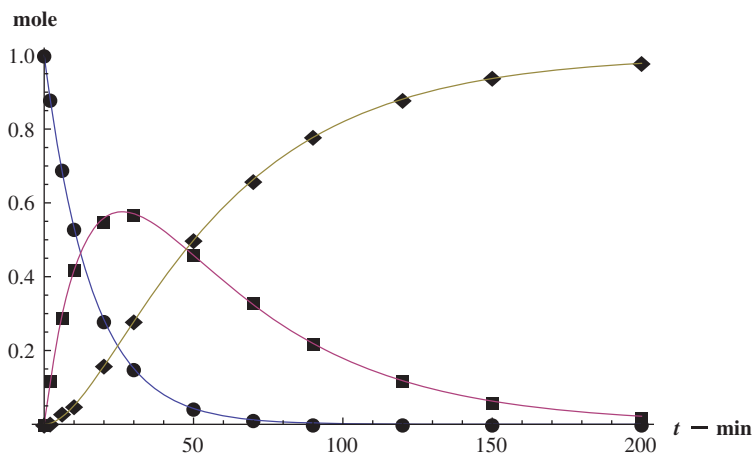


Figure 6. A plot of the amounts of A (●), B (■) and C (◆) as a function of time in minutes with the solution to the differential equations model using the parameters $k_1 = 0.0629595$ and $k_2 = 0.0211523$ obtained from the least square approach. We see an excellent fit.

the following parameter values $k_1 = 0.0628918$ and $k_2 = 0.0210947$, and we note the slight difference in these values as compared to those obtained when using all three sums for A, B and C data. Such variations in parameters give essentially the same fit and plots for Figure 6.

3.3. Sensitivity of parameters

In Figure 7, we show the results of solving the differential equation system describing our chemical reaction in two cases, using values of our estimated parameters which are (1) 20% higher and (2) 20% lower than our optimal estimates. We note the band surrounding the actual observations and suggest that even a 20% error in our parameter estimates renders a reasonable prediction for the reaction.

Another examination of sensitivity is to consider the fact that there could be ‘noise’ in the data and we should determine how sensitive our algorithm is to estimating our parameters k_1 and k_2 in light of this noise. We run 2000 simulations in which we put random noise into our data. We do this by taking each observation, say $x(t)$ to represent one of $a(t)$, $b(t)$, or $c(t)$, at each time, t , and converting $x(t)$ to a data point $x(t) \cdot (1 + \varepsilon(t))$ where $\varepsilon(t)$ is a random number from a normally distributed random variable with mean $\mu = 0$ and variance $\sigma^2 = 0.01$.

In each of these simulations we obtain best values for k_1 and k_2 using our sum of square error over all three chemical observations for the time observations we have. We plot our 2000 results for k_1 and k_2 in a histogram in Figures 8 and 9, respectively. The average k_1 value for the 2000 estimates is $\hat{k}_1 = 0.0636118$ which is very close to our initial estimate, $k_1 = 0.0629595$, and in the case of k_2 we obtain an average $\hat{k}_2 = 0.0212466$ which is very close to our initial estimate, $k_2 = 0.0211523$. This suggests that if we were to do this parameter estimate process with noisy data (we call this real-life!) that we would get parameters quite close to our original optimal values of k_1 and k_2 . Of course, if we were to have exceptionally noisy data, say $\sigma^2 = 0.1$ we

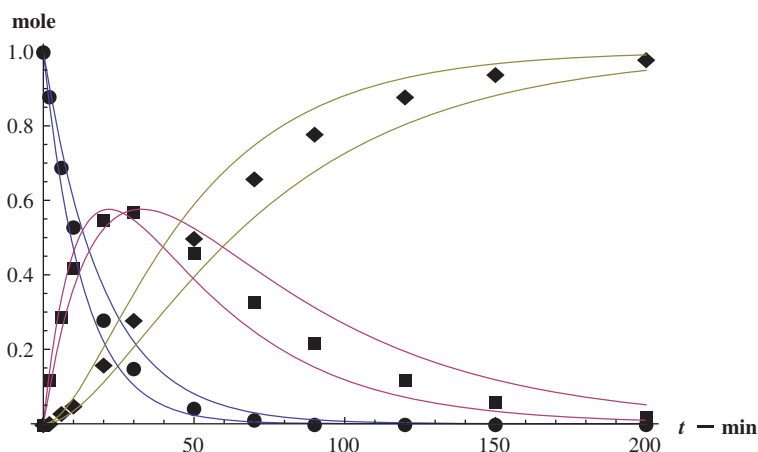


Figure 7. A plot of the amounts of A (●), B (■) and C (◆) as a function of time in minutes with the solution to the differential equations model using both a 20% increase and a 20% decrease in the parameters $k_1 = 0.0629595$ and $k_2 = 0.0211523$ obtained from the least square approach. We see for each chemical a reasonable band about the actual observations reflecting these changing parameter values.

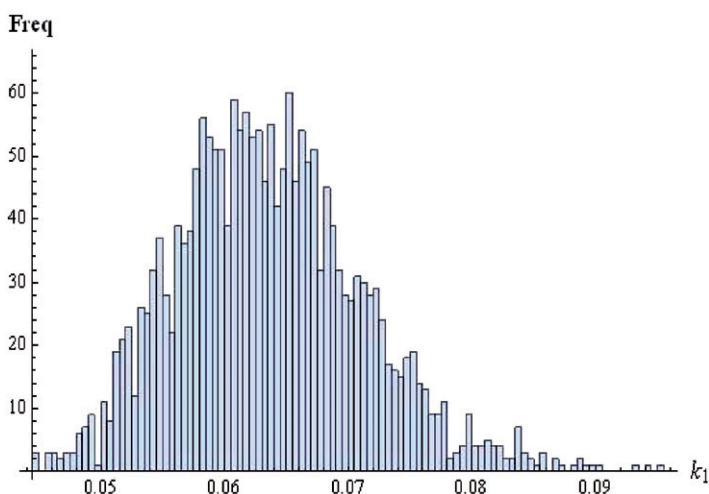


Figure 8. A histogram of best values of parameter k_1 from 2000 simulations in which we added random noise to the values of our chemical observations for A, B and C for each data point in the form of a deviate from a normally distributed random variable with mean, $\mu = 0$ and variance, $\sigma^2 = 0.01$.

would have a much wider spread in our histograms and thus the chance of greater variation in our estimates.

We see our method gives a robust approach to estimating the parameters k_1 and k_2 successfully when the observational data offered up is not too noisy. Moreover, there is only slight sensitivity in our estimates for k_1 and k_2 to small changes in the values in the observed data.

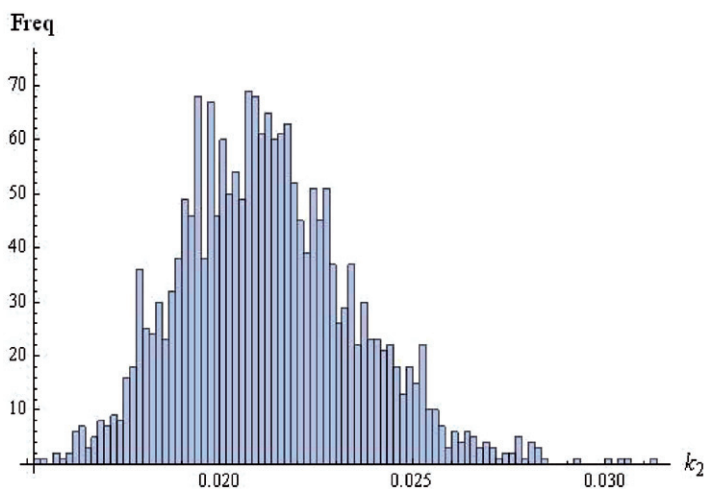


Figure 9. A histogram of best values of parameter k_2 from 2000 simulations in which we added random noise to the values of our chemical observations for A, B and C for each data point in the form of a deviate from a normally distributed random variable with mean, $\mu = 0$ and variance, $\sigma^2 = 0.01$.

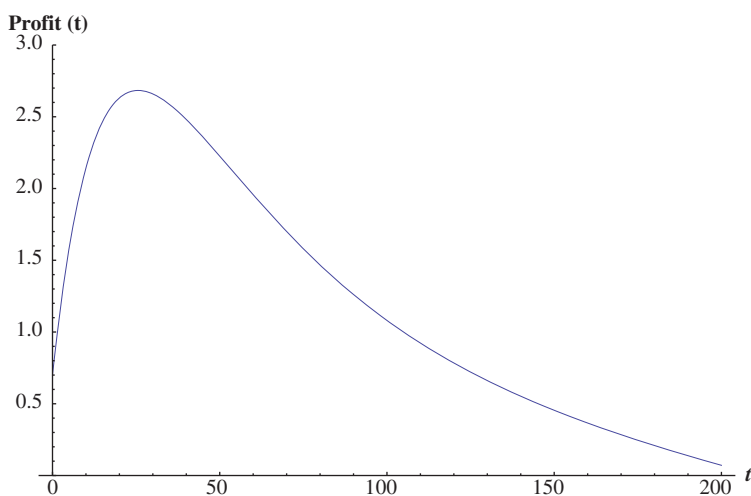


Figure 10. A plot of the profit function using the recovered functions for the amounts of A, B and C, at time t and the running cost of operating the reaction.

3.4. Optimizing profit

Thus far we have solved the kinetics portion of the effort and we turn to the optimization problem. We seek to maximize profit given running time costs, purchase costs and recovered material revenue (see Figure 10).

$$\begin{aligned} \text{Profit}(t) &= 0.75 - 0.005t + 0.05a(t) + 3.5b(t) + 0.25c(t) \\ &= 1 - 0.005t - 5.19434e^{-0.0629595t} + 4.89434e^{-0.0211523t} . \end{aligned}$$

Using calculus we recall that the optimum for Profit(t) occurs when Profit'(t) = 0, so we have *Mathematica* do this for us:

```
solMaxProfit = FindRoot [Profit'[t]==0, {t,25}]
```

to obtain $t_{\max} = 25.6053$ with a maximum value of Profit(t_{\max}) = 2.68344. We have now completely solved our kinetics problem and our optimization problem.

4. Conclusion

We have shown how the study of differential equations can be motivated and the modelling process for building differential equations which describe chemical kinetics according to the law of mass action can permit parameter estimation studies and thus a completion of the modelling cycle with validation of our model for our given data for differential equation activities involving data and realistic situations. We have used this approach in courses in which we have just introduced differential equations, indeed, before solution strategies for differential equations have been addressed as we have the benefit of *Mathematica*'s DSolve command. We have used these approaches and problems in every modelling course we have taught. In all cases we found the students fascinated by the application of the mathematics they were studying to a course they took, often concurrently. Moreover, students became familiar with several processes which would enable them to estimate parameters in differential equations models, something they might not experience until much later in their education, if ever at all! We highly recommend you make every effort to incorporate such parameter estimation strategies in your course for the sake of your students, for they need to see the 'end game' of modelling as well as the model formulation and the techniques associated with solving differential equations.

Note

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