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Mathematical models for chemistry and biochemistry service courses

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In this paper, applications and modelling problems for chemistry and or biochemistry courses are analysed. They obtain better results than others, in order to motivate students of chemical careers towards mathematical problem solving, since these problems are specially tailored for their needs. A teaching experience, carried out during two decades is analysed and a particular example is exposed with further details. The results of this experience led us to several conclusions that are included in the last section of the article.

Keywords: Nonlinear models, chemical careers, students’ motivation.

INTRODUCTION

In chemical careers mathematical courses like numerical methods, differential equations and statistics are widely used to solve problems concerned with modelling real problems relevant for chemistry and/or biochemistry. Nevertheless, most mathematical texts include only physical problems more relevant for other disciplines, like mechanics or electromagnetism. The need for relevance was highlighted by many writers as being important in motivating students when learning mathematics. For example, Bajpai, Mustoe and Walker (1975) suggested a range of improvements including a modelling approach and providing more relevant examples. In the same direction, according to McAlevey and Sullivan (2001), there is a need for using real-life problems since ‘Students are best motivated by exposure to real applications, problems, cases and projects’.

For this reason, several previous articles (Martinez-Luaces, 2003, 2006, 2009a) have focused on how modelling may be used to motivate students in those careers. In particular, ordinary differential equations (O.D.E.) linear systems appear regularly in Chemical Engineering, Food Technology Engineering and Environmental Engineering courses. This is due to the usefulness in modelling chemical kinetics (Martinez-Luaces, 2012a), or water solutions, mixtures and reactors problems (Martinez-Luaces, 2005).

The introduction of chemical and/or biochemical problems help to motivate students and can be widely used for modelling and applications examples, particularly in differential equations (Martinez-Luaces, 2006), probability and statistics (Martinez-Luaces, Velazquez, & Dee, 2009) and numerical methods (Guineo Cobs & Martinez-Luaces, 2003).

In previous papers and in a pair of books (Martinez-Luaces, 2009b, 2012b), problems involving chemical kinetics, mixing problems, reactors, etc. have been exposed and analysed from its educative potential viewpoint. In this paper, more simple models will be considered and a concrete example will be discussed in the third section. Despite the simplicity of these models, they appear regularly in several branches of chemistry and biochemistry; they allow teachers to pose interesting questions and even project work to be carried out by the students in small groups.

Conclusions based on the results of the teaching methods used, will be drawn for differential equations, statistics and numerical methods courses for chemical careers. Several of these conclusions can be easily extrapolated to other mathematical service courses.

A PARTICULAR EXPERIENCE IN URUGUAY

In the late 90’s, a small group of teachers and researchers was formed in the Chemistry Faculty at the University of the Republic of Uruguay (UdelaR), having their members an applied profile. For sever-
al years, this team included chemists, engineers and applied mathematicians. This group – in addition to other tasks as mathematical and engineering consultants – was appointed to be in charge of a course called Mathematics III, created in 1996 especially for Food Engineering students. The original syllabus included Ordinary Differential Equations (ODE), Partial Differential Equations (PDE) and an introduction to Laplace Transform, with emphasis towards applications and other disciplines. After the change of plans in year 2000, this course was replaced by another two – Mathematics 005 for Food Technology Engineering and Mathematics 105 for Chemical Engineering – with more class hours per week and a greater presence of modelling activities and applications.

Since the beginning of this course, direct and inverse modelling problems were proposed to the students (Martinez-Luaces, 2009a). Three thematic areas were especially suitable for this purpose: Chemical Kinetics (Martinez-Luaces, 2012a), mixing problems (Martinez-Luaces, 2009b) and Mass Transfer (Martinez-Luaces, 2003).

Chemical Kinetics is an important source for interesting problems. In our research work, the most refined versions of those problems were published in books, papers and proceedings, such as: Guineo Cobs and Martinez-Luaces (2002), Martinez-Luaces (2005, 2009b, 2012a, 2012b). Examples of these problems are: mutarotation of glucose, mechanisms with two or three reactions in series, carbon dioxide adsorption on platinum surfaces, etc.

Mixing problems have been another important source for modelling problems, such as: interconnected tanks system, tank divided into several compartments, stirred tank with recirculation, etc. These problems and many others have been included in papers published in international journals (Martinez-Luaces, 2005, 2009a), in books (Martinez-Luaces, 2009b, 2012b) and conference proceedings (Martinez-Luaces & Alfonso, 2000; Martinez-Luaces, 2007).

Finally, with regard to the problems involving parabolic PDE applied to Mass Transfer real situations, there are many examples that can be mentioned. For instance: drying a vegetable through its faces, sugar diffusion in a cherry, chives drying process, dissolved oxygen electrode, packed bed chemical reactor, diffusion of pollutants in the Chernobyl accident and pollution in the Rio Uruguay. These problems were presented briefly – with its analytical and/or numerical solution discussed – in an article published in New Zealand Journal of Mathematics (Martinez-Luaces, 2003), but there are also full versions of the modelling process with further details of the resolution in a book published a few years later (Martinez-Luaces, 2009b). Partial preliminary versions of those problems were presented in mathematical education conferences like Martinez-Luaces and colleagues (2000, 2001), Guineo Cobs and Martinez-Luaces (2003) and Martinez-Luaces and Guineo Cobs (2005), among others.

A NONLINEAR MODEL USEFUL FOR CHEMICAL CAREERS

The nonlinear mathematical formula \( y = \frac{a x}{x + b} \) (Eq. 1) is widely used in chemistry and biochemistry for different purposes. For instance, the Michaelis-Menten kinetics is a well-known model in biochemistry of the form \( v = \frac{v_{max} [S]}{K_m + [S]} \) (Eq. 2) where \( v_{max} \) and \( v_{max} \) are the initial and the maximum velocity of the enzymatic reaction, \([S]\) is the substrate concentration and \(K_m\) is a constant (called Michaelis constant), which depends on the enzymatic reaction considered (Nelson & Cox, 2008).

Irving Langmuir, a Nobel Prize winner in chemistry, developed an equation that relates the coverage or adsorption of molecules on a solid surface to gas pressure or concentration of a medium above the solid surface at fixed temperature (Masel, 1996). The equation is \( \Theta = \frac{a x}{1 + a P} \) (Eq. 3) where \( \Theta \) is the fractional coverage of the surface, \(P\) is the gas pressure (or concentration in the case of liquids) and \(a\) is a constant. A very simple algebraic manipulation gives \( \Theta = \frac{P}{a x + P} \) (Eq. 4) which is just a particular case of (Eq. 1).

The last example is a mathematical model for the growth of microorganisms proposed by Jacques Monod (1949). The mathematical formula is \( \mu = \frac{\mu_{max} S}{K_s + S} \) (Eq. 5), where \( \mu \) is the specific growth rate of microorganisms and \( \mu_{max} \) represents its maximum value, \( S \) is the concentration of limiting substrate for growth and \( K_s \) is called the “half-velocity constant” (Martinez-Luaces, 2009b), since it corresponds to the value of \( S \) when \( \frac{\mu}{\mu_{max}} = \frac{1}{2} \) as well as the constant \( K_m \) in (Eq. 2).

The Monod equation has the same form as the Michaelis-Menten equation, but it was developed
empirically whereas the Michaelis-Menten model is based on theoretical considerations.

A typical problem that arises in the treatment of data corresponding to these equations is the parameters determination since all of them are nonlinear models. In order to solve this problem, several methods were proposed to linearize these equations, being Lineweaver-Burk, Hanes-Woolf, Eadie-Hofstee, Scatchard, and Eisenthal-Cornish-Bowden the most important ones (Nelson & Cox, 2008).

For instance, the Lineaweaver-Burk (or double reciprocal plot method), proposes a graphical representation of $\frac{1}{V_0}$ vs $\frac{1}{S}$. It is easy to observe that the reciprocal of (Eq. 2) gives $\frac{1}{V_0} = \frac{K_M}{V_M} \frac{1}{S} + \frac{1}{V_M}$ (Eq. 6), so the $x$–intercept of the graph represents $-\frac{1}{K_M}$ and the $y$–intercept is equivalent to the inverse of $V_M$. An alternative way is to obtain the coefficients of a linear regression (i.e. $\frac{K_M}{V_M}$ and $\frac{1}{V_M}$) and finally get $K_M$ and $V_M$ from these coefficients.

Other methods propose a different linearization or another mathematical procedure for recovering $K_M$ and $V_M$ from experimental data.

All these methods can be compared in terms of exactitude and precision (Martinez-Luaces & Silva, 2014), using simulated data perturbed with Gaussian noise with different amplitudes. This comparison is particularly significant when the relation between trend and noise tends to increase.

Since equations (2), (3) and (4) represent the same mathematical model (Eq. 1), one of them (the Michaelis-Menten equation) may be chosen as an example in order to show the methodology to be followed.

In the selected equation, the parameters are $K_M$ and $V_{\text{max}}$ and variables are $[S]$ and $v_0$. In a previous paper (Op. cit., 2014), typical values of these parameters and variables were chosen and theoretical curves were obtained. A Gaussian noise with different amplitudes was superimposed to the theoretical data obtained from (Eq. 2) with typical values of $V_M$, $K_M$ and $[S]$.

The graphics in Figure 1 show the simulated curves for the Michaelis-Menten equation (initial velocity vs substrate concentration) with the Gaussian noise multiplied by coefficients 1, 2, and 3, respectively.

![Figure 1: Simulated data for the Michaelis-Menten equation](image)
These simulated data took the place of the real experimental data and were used to determine the parameters $K_M$ and $V_M$, which real values were known, so the different methods were easily compared in terms of exactitude and precision. Table 1 shows the minimum absolute and relative errors in $K_M$ and $V_M$ and which methodology was the best in each case, depending on the noise amplitude.

The method due to Eisenthal and Cornish-Bowden (CBE in Table 1) was the best one in all the cases, except when the Gaussian noise had double amplitude and $K_M$ is the considered parameter. In this last case, Eadie and Hofstee’s method (H in Table 1) obtained the minimum absolute and relative error in the parameter $K_M$, but not in $V_M$ where once again Eisenthal and Cornish-Bowden gave the best estimate.

A similar methodology was followed in another article devoted to Electrochemical Noise studies (M. Martinez-Luaces, V. Martinez-Luaces, & Ohanian, 2006).

### RESULTS

Modelling was introduced in UdelaR Statistics and Differential Equations courses for Chemical Engineering and related careers in 1996. Since then, modelling and application problems regularly appeared in final examinations and other forms of assessment. A similar situation took place in other subjects like Design of Experiments and Numerical Methods, as it was analysed in previous papers (Martinez-Luaces, 2005, 2009a; Martinez-Luaces et al., 2009).

Throughout this teaching experience, as it was already remarked, modelling problems and applications were not just discussed in class, but they also played an important role in the assessment. This is a very important issue, for example Smith and Wood said that “...appropriate assessment methods are of major importance in encouraging students to adopt successful approaches to their learning. Changing teaching without due attention to assessment is not sufficient” (Smith & Wood, 2000).

In this experience with students of Chemical Engineering and Food Technology Engineering, several surveys of student opinions were conducted through anonymous questionnaires. The transcribed below are some of the students’ responses to those semi-open questionnaires; they reflect a very positive attitude towards the courses themselves and the problems proposed during those courses:

> Now I find that mathematics can be useful.
> A really super course, I got a great deal out of it.
> An interesting course, with quite a lot of applications in real life.

Specifically, about tasks related to modelling and applications, they had this to say:

> If these topics were omitted, the course would just be another standard maths course, a ‘hard’ subject filled only with methods, calculations and numbers.

Once the new study plan was started, the course known as Mathematics III was replaced with Mathematics 005 and 105. After these changes, the students were again consulted by means of semi-open questionnaires. These are some of their views:

> Very directly applicable to my undergraduate professional career; it renewed a taste for mathematics and it was well taught, guiding the solutions to the exercises and not working them all out.

### Table 1: Comparison of the results for the different methods

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<tbody>
<tr>
<td>Amplitud Noise 1</td>
<td>0.0167</td>
<td>0.3243</td>
<td>0.0017</td>
<td>0.0032</td>
<td>CBE</td>
<td>CBE</td>
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<td>0.0088</td>
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<td>H</td>
<td>CBE</td>
<td>H</td>
<td>CBE</td>
</tr>
<tr>
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<td>1.4027</td>
<td>0.0394</td>
<td>0.0140</td>
<td>CBE</td>
<td>CBE</td>
<td>CBE</td>
<td>CBE</td>
</tr>
</tbody>
</table>
I thought the course was very useful and dynamic, and I think it will have very useful applications in coming years.

As for the modelling, applications, and the problems set, these were some of their comments:

The problems were motivational because you can see the usefulness of mathematics in daily life, and they clearly show the interaction that exists with other subjects.

I have taken courses in which the applications dealt with here were relevant.

Very useful examples for future years of undergraduate study.

As can be seen, the students reacted very positively not only to the course they were taught (before and after the initiation of a new study plan), but also in particular, within the course, they appreciated everything to do with the problems, involving modelling and applications.

The statistical results of these surveys – published in Martinez-Luaces (2009a) – confirm those views corresponding to several selected opinions.

CONCLUSIONS

The main goals of the activities described in the previous sections are both technical and educative. From the technical viewpoint the results obtained with simulated data showed that the method most widely used (Lineweaver-Burk) it is not the most accurate and this fact constitutes a surprising result for the majority of the students. From the mathematical education viewpoint students’ positive reactions can be explained in terms of the following characteristics of the studied problems:

a) relevance
b) applicability
c) specificity
d) authenticity
e) low pre-requisites

The need for relevance was specially remarked in the discussion at CERME9, TWG06. The example considered above is especially relevant for students of several careers such as Chemistry, Biochemistry, Chemical Engineering, Food Technology Engineering and Environmental Engineering. The problem relevance – at least in this case – is linked with the problem applicability and its specificity. The results showed that students usually react more positively to these problems than to other application problems which are not so specific (like problems about circuits or mechanics, etc.).

Other issue that was widely discussed in the TWG06 was the need of authenticity for the modelling activities. In this case not only the models are real models, even more, the methods for recovering parameters are the “real ones”, in the sense that these are the methods that the students will use in other subjects like Biochemistry, Microbiology and Physical Chemistry.

Last but not least, pre-requisites are an important constraint when choosing modelling and application activities. The problem described above and the corresponding linearization methods have very low pre-requisites and they only need some algebraic manipulations to be understood. For the proposed activities (i.e., the data simulation and the recovery of the parameters) the students only need a previous course in Probability and Statistics and some basic skills when using MATLAB® or any other software.

It is important to remark that very simple mathematical models, like the one discussed above, are excellent sources for this kind of problems. Moreover, there exists an important set of real-life problems from these areas, which remain almost unexplored from the point of view of their mathematical education richness.

Searching for new real-life problems to be used for project-work in chemical and biochemical careers represents an interesting challenge for mathematical education researchers. At the same time, it provides a good opportunity for an interdisciplinary work with teachers and researchers from other disciplines with the resulting benefits.

REFERENCES


