Modelling, applications and inverse modelling: innovations in differential equations courses

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Abstract: Differential equations and Laplace transform are widely used to solve problems concerned with mathematical modelling and applications. These analytical tools appear regularly in chemical engineering courses, due to the usefulness in modelling chemical kinetics, mixing problems and reactors design, among other problems. The discussion in this paper will deal with non typical inverse problems and how they can be used in engineering courses. Recommendations will be drawn for undergraduate courses in differential equations for chemical engineering and other related careers.

Keywords: Modelling and applications; Differential Equations; Engineering courses; Inverse problems

2000 Mathematics Subject Classifications: 97D50; 34A30; 34A55

1. Introduction

Modelling and application is nowadays an important and fast growing area in mathematics education at the tertiary level. On the other hand, differential equations (both ordinary and partial) and Laplace transform (abbreviated as O.D.E., P.D.E. and L.T. in what follows) are mathematical tools that since their beginning are strictly related with applications in other sciences and engineering.

These mathematical tools (i.e., O.D.E. and L.T.) are very useful when mixing problems are considered [1] and [2]. Moreover, as it was commented in other papers and books [2-3], a stirred tank system can, under certain conditions, be considered as a chemical reactor. For instance, under ideal conditions, a stirred tank is a “Continuous Stirred Ideal Reactor” (CSIR) [4]. This fact was mentioned, and analysed in [2-3-5], among other publications.

As a consequence, mixing and/or chemical reactor design problems are excellent sources for applications and modelling examples where O.D.E. and L.T. are widely used.

When mixing problems are included in differential equations texts, volume, geometry and flux data of the tanks are given and so, a trained student can solve such problems just as an exercise. Once they have solved a “typical set” of these problems, they become a routine task, which is interesting from the applications view point, but is no longer a problem to challenge students.

The inverse problem corresponding to the typical mixing situation, consisting in asking which tank system, if any, corresponds to a given function or a given O.D.E. linear system. As it is usual in inverse problems [6-7], the desired conditions of existence, uniqueness and stability are not present in many cases. This kind of
problem—called inverse modelling problems in previous papers [2-4-5]—is more interesting due to its mathematical richness and unpredictability. As was shown in other papers [2-4-5], inverse modelling situations related to stirred tanks and reactors, cannot always be solved, or there may not be a unique solution but even in this case, slight modifications in functions or O.D.E. coefficients produce big changes in the final results.

In the next section some new problems (not analysed in other papers), will be considered, taking into account their potential richness from a mathematical education viewpoint.

2. Several inverse modelling problems

a) Previous concepts

The following ideas and concepts are included near the beginning of any O.D.E. and L.T. course.

i) An ideal stirred tank:

A stirred tank (CSIR reactor) is showed in the following figure:

![Ideal stirred tank](image)

Figure 1 Ideal stirred tank

In this problem, the input is a water solution of salt with a volumetric flux $\Phi$ (L/s) and a concentration $C_0$ (g/L). The volume of the tank is $V$ (L).

If $\Phi$ and $V$ are constants, then: $V \frac{dC}{dt} = \Phi C_0 - \Phi C \quad C(0)=0$

Applying L.T. we have: $V (s L[C] - C(0)) = \Phi L[C_0] - \Phi L[C]$

And rearranging we get: $L[C] \cdot (V \cdot s + \Phi) = \Phi \cdot L[C_0]$
The transference function is defined as: $G(s) = \frac{L}{L} \left[ \frac{C(t)}{C_0(t)} \right]$, i.e., the quotient between L.T. applied to the output and input and it is a characteristic of the reactor.

In this case we have: $G(s) = \frac{\Phi}{V_s + \Phi}$

Rearranging again and putting $\frac{V}{\Phi} = \tau$, the result is: $G(s) = \frac{1}{1 + \tau s}$, where $\tau$ is the average time of a water molecule in the reactor.

ii) Reactors in series and parallels:

Using the definition given for the transference function, then for a series of two chemical reactors (see figure 2), it is easy to obtain the following formula:

$$G(s) = G_1(s)G_2(s)$$

![Figure 2. Series of two chemical reactors.](image)

It is possible to obtain a general version for a series of $n$ chemical reactors.

A little more difficult is to derive the formula for a parallel system consisting of a pair of chemical reactors as in the following figure:

![Figure 3. Parallel of two chemical reactors.](image)

In this case, a mass balance at the second bifurcation point, and several algebraic manipulations give:

$$G(s) = \frac{\Phi_1}{\Phi} G_1(s) + \frac{\Phi_2}{\Phi} G_2(s) = f_1G_1(s) + f_2G_2(s),$$

where the coefficients $f_i$ are $f_i = \frac{\Phi_i}{\Phi}$, so they can be interpreted as fractions of total...
flux. This formula can be easily generalised to give \( G(s) = \sum_{i=1}^{n} f_i G_i(s) \), where \( \sum_{i=1}^{n} f_i = 1 \) for obvious reasons.

b) Two little theorems:

In this second part, two theoretical results will be stated:

i) A series of \( n \) ideal stirred reactors:

A series of \( n \) CSIR reactors is considered, as in the following figure:

![Figure 4. Series of n CSIR.](image)

In this case, it is easy to get the following formula:

\[
G(s) = \frac{1}{1+\tau_1 s} \cdots \frac{1}{1+\tau_n s} = \frac{1}{(\tau_1 \cdots \tau_n) s^n + \cdots + 1}
\]

Moreover, it can be seen that \( G(s) = \frac{1}{a_n s^n + \cdots + a_i s + 1} \), where \( a_n = \prod_{i=1}^{n} \tau_i \)

and \( a_i > 0 \ \forall i \).

As a theoretical exercise, students can be asked to demonstrate this result using complete induction.

ii) A parallel of \( n \) CSIR:

As usually happens, the parallel equivalent is not so easy as the series example. For instance, if only two CSIR are considered, it follows that:

\[
G(s) = f_1 \frac{1}{1+\tau_1 s} + f_2 \frac{1}{1+\tau_2 s}
\]

being \( f_1 = \frac{\Phi_1}{\Phi_1 + \Phi_2} \) and \( f_2 = \frac{\Phi_2}{\Phi_1 + \Phi_2} \). Then, in this case, the transference function is:

\[
G(s) = \frac{(f_1 \tau_2 + f_2 \tau_1)s + (f_1 + f_2)}{\tau_1 \tau_2 s^2 + (\tau_1 + \tau_2)s + 1}
\]

The expression \( f_1 \tau_1 + f_2 \tau_2 \) is positive and, at same time, it is a convex linear combination of residence times \( \tau_1 \) and \( \tau_2 \), while the other coefficient \( f_1 + f_2 \) is

\[
f_1 + f_2 = \frac{\Phi_1 + \Phi_2}{\Phi} = \frac{\Phi}{\Phi} = 1
\]

Once more these results can be generalised for a parallel of \( n \) CSIR reactors, as in the following figure.
In this case it is possible to get \( G(s) = \frac{b_{n-1}s^{n-1} + \cdots + b_1s + 1}{a_ns^n + \cdots + a_1s + 1} \) where \( a_ns^n + \cdots + a_1s + 1 \) is the same as in the series case, \( b_j > 0 \ \forall j \) and the first coefficient \( b_{n-1} \) is a convex linear combination of \( \tau_1 \cdots \tau_{n-1}, \ldots, \tau_2 \cdots \tau_n \) (i.e., all the \( n-1 \) factors product of residence times).

Another possibility consists in writing
\[
b_{n-1} = \left( \prod_{i=1}^{n} \tau_i \right) \cdot \left( \sum_{i=1}^{n} \frac{f_i}{\tau_i} \right).
\]

As in the series case, all these results can be demonstrated by induction and this can be a theoretical exercise for the students.

c) Consequences of the previous results:

Interesting inverse modelling problems can be put to the students. For example, this function can be considered: \( G(s) = \frac{s^2 + s + 1}{(1+s)(1+2s)(1+3s)} \). Does it correspond to a parallel of CSIR? In a heuristic approach the answer may be “yes”, but analysing the previous results shows it to be impossible. This fact can be observed by taking into account that \( G(s) = \frac{P(s)}{Q(s)} \), where \( Q(s) = (1+s)(1+2s)(1+3s) \) suggest to consider three CSIR with residence times \( \tau_1 = 1, \tau_2 = 2, \) and \( \tau_3 = 3 \). Nevertheless, in this case \( \tau_1\tau_2 = 2, \ \tau_1\tau_3 = 3, \) and \( \tau_2\tau_3 = 6 \), so the first coefficient of \( P(s) \) must
be between 2 and 6, because this coefficient must be a convex linear combination of the two-factors products. This is not the case, because \( P(s) = s^2 + s + 1 \) and so, the function considered \( G(s) = \frac{s^2 + s + 1}{(1 + s)(1 + 2s)(1 + 3s)} \) does not correspond to a parallel of CSIR.

Even more, not all the convex linear combinations are allowed. For example \( G(s) = \frac{3s^2 + 4s + 1}{(1 + s)(1 + 2s)(1 + 3s)} \), seems to be a parallel of three CSIR, but it is not the case. After simplifying this quotient, it can be reduced to: \( G(s) = \frac{1}{1 + 2s} \) (just one reactor with \( \tau_2 = 2 \)).

Slight changes in the first coefficient can give: \( G(s) = \frac{3.02s^2 + 4s + 1}{(1 + s)(1 + 2s)(1 + 3s)} \), which corresponds to a parallel system with \( f_1 = 0.01 \), \( \tau_1 = 1 \), \( f_2 = 0.98 \), \( \tau_2 = 2 \) and \( f_3 = 0.01 \), \( \tau_3 = 3 \), or modifying again the first coefficient in the other sense \( G(s) = \frac{2.98s^2 + 4s + 1}{(1 + s)(1 + 2s)(1 + 3s)} \) which does not correspond to a parallel of CSIR (the last statement can be proved by a decomposition in simple fractions).

### 3. The mathematical education viewpoint

The examples already analysed (and/or others of the same kind) can be proposed as an interesting complement to traditional mixing problems. The typical mixing problem includes tanks, chemical solutions, fluxes, etc., and the main purpose is to write an O.D.E. linear system and to solve it. Taking into account the results and ideas of section 2, there are other possibilities, such as the following ones:

1. Apply L.T. and consider the tank system as a chemical reactor (this idea was already exploited in [1]).
2. Try to describe the reactor as a series and/or parallel of ideal reactors and ask the students if a solution exists, if it is unique and if it is stable under slight modifications (these questions were analysed in [2-4-5]).
3. Ask the students to prove (using complete induction, simple fractions, etc.) theoretical results about series, parallels and combinations of both (examples of such theoretical results were shown in the previous section, but there are others that can be used).
4. Finally, ask the students if given formulas (rational fractions for example) can be considered as the transference function of an ideal reactor or not. In the case of a positive answer, it can be asked if the reactor is the unique one and/or what happens if slight modifications in the coefficients are made.

These modifications, among others (for example, consider other kinds of reactor, recirculation, mix of series and parallels, etc.) can convert the typical mixing problem –which works more as an exercise for experienced students– in a real problem whose solution is not obvious.

The main idea is to substitute –or at least complement– routine exercises with real problems which imply an interesting challenge for engineering students.
4. Modelling and inverse problems in our courses

Modelling was introduced in U.D.E.L.A.R. differential equations courses for chemical engineering and related careers courses in 1996, and since then, mixing problems have appeared in the final examinations [1-5]. Inverse problems appeared in the assessment of this course, two years later in 1998. The questions had two different settings: firstly, tank dimensions and geometry were given, and students were asked to obtain an input for a desired output; and secondly, both input and output were given and the question was about what to put in the middle (i.e., how many tanks, which volumes and fluxes, what connections occurred between them, etc.). Finally, inverse-modelling issues were considered specifically since year 2005 [2-8-9], although inverse-modelling students’ questions, appeared since the beginning of all this experience, in 1996 [5].

As it was mentioned before, all this teaching experience incorporated modelling, problem-solving and inverse-modelling. All of them were not just discussed in the classes, but played an important part of 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” [10].

5. Results

In several faculties (Engineering, Chemistry, Sciences, etc.) at U.D.E.L.A.R., the Education Department evaluates teachers, courses, assessment procedures (exams, etc.) by asking for students' opinion through questionnaires. The most typical questionnaire is composed of 25 questions using a Likert scale as follows:

<table>
<thead>
<tr>
<th>Likert Scale</th>
<th>Score</th>
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<tbody>
<tr>
<td>Total agreement</td>
<td>10</td>
</tr>
<tr>
<td>Partial agreement</td>
<td>7.5</td>
</tr>
<tr>
<td>Indifference</td>
<td>5</td>
</tr>
<tr>
<td>Partial disagreement</td>
<td>2.5</td>
</tr>
<tr>
<td>Total disagreement</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1. Likert scale used in the questionnaire.

From this set of twenty-five questions, seven are particularly relevant and important to evaluate the inclusion of modelling and inverse modelling issues in differential equations courses. These questions are:

1) The pitch and pace of class can be followed by the students
2) The examples presented in the classroom illustrate the courses' main concepts.
3) Relationship with other subjects is established.
4) An applied approach is developed, giving examples and applications connected with real-life problems and professional practice.
5) Students are motivated in this course.
6) Students feel comfortable and enjoy classes.
7) Final exams and assessment problems and exercises can be solved using knowledge obtained in class.

Table 2 compares the average scores for the seven questions in both the innovative experience (group A, i.e., lecturers of the differential equations courses), with the other two traditional groups (group B and group C, corresponding to other mathematical courses of the same department).

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
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<tbody>
<tr>
<td>A</td>
<td>9.27</td>
<td>9.52</td>
<td>8.87</td>
<td>9.03</td>
<td>8.39</td>
<td>8.47</td>
<td>8.75</td>
</tr>
<tr>
<td>B</td>
<td>7.88</td>
<td>8.00</td>
<td>7.50</td>
<td>6.44</td>
<td>6.50</td>
<td>7.31</td>
<td>7.56</td>
</tr>
<tr>
<td>C</td>
<td>6.94</td>
<td>6.48</td>
<td>4.22</td>
<td>4.19</td>
<td>5.16</td>
<td>5.58</td>
<td>4.90</td>
</tr>
</tbody>
</table>

Table 2. Comparison between "innovative" and "traditional" groups.

Group A teachers' assessment can be compared in two different situations: before 1996, when the innovative experience started, and after 1996, i.e., after including modelling and inverse modelling problems. This comparison can be observed in the following average scores:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
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<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before 1996</td>
<td>8.45</td>
<td>8.87</td>
<td>8.20</td>
<td>7.61</td>
<td>8.63</td>
<td>8.57</td>
<td>-</td>
</tr>
<tr>
<td>After 1996</td>
<td>9.27</td>
<td>9.52</td>
<td>8.87</td>
<td>9.03</td>
<td>8.39</td>
<td>8.47</td>
<td>8.75</td>
</tr>
</tbody>
</table>

Table 3. Group "A" teachers' assessment before and after including modelling and inverse modelling problems. Average scores.

A comparison of the teaching style is possible before and after the innovative experience respectively, since teachers of the group “A” (i.e., four professors involved in the differential equations course) taught equivalent students both times (engineering courses, first O.D.E. course, etc.).

There are other issues that must be commented:

a) Question 7 was not included in the questionnaire before 1996, so, there is no result in the corresponding row in table 3.
b) The mean scores in questions 5 and 6 diminished slightly, this may be due to the dramatic increase in the number of students between 1993 and 1996.
c) It follows from Table 3, that the first four questions showed an important mean score increase. Moreover, if questions 1 to 6 are considered, there exists an average increase of 6.65 %, which is very important, because this improvement was obtained teaching the same syllabus plus an extra subject (chemical kinetics and mixing problems among other applications problems).
d) Teachers involved in this innovative experience achieved the best results in motivation (question 5).

All these results were reinforced by several students' comments about different topics as applications, motivation, etc. Several examples are the following sentences:
Student I: "I never thought that Maths had so many applications related with my career"
Student II: "Teachers help us in solving real-life problems, but they don't do all the task...we must work hard...this is the best way to learn"
Student III: "All Maths courses should be like this"

Another interesting consequence of this innovative approach was the improvement in comprehension when students had their second experience with this kind of problems in other subjects (Physical Chemistry, Design of Reactors, etc.) of their careers. We have remained in contact with many former students through other activities, and they continue to report that they are using skills and knowledge that they acquired through our courses. This fact is in concordance with the experiences of other teachers in other parts of the world, when courses are based on problem-solving activities [11].

In a previous paper, an expert group was consulted, and almost all the experts remarked the importance of teaching significant concepts and procedures in service courses. From a different point of view, engineering students showed an important preference for teachers who make the effort of presenting real-life problems, related with their own careers [12].

Finally, cluster analysis and other multivariate statistical methods showed a very similar situation [13]. More precisely, in our group of mathematical teachers (twelve teachers in the Mathematics Department), the cluster analysis of "applications" separate a group of them as the better ones. It is important to mention that this variable "applications" consists of a 12-components vector with the average results of two questions: the one related with real-life problems (question 4) and the other about the connection with other disciplines (question 3). The group with the best results (a group of five teachers) was integrated almost exclusively with differential equations' teachers.

It is important to note that almost all of these teachers (the ones with better results in "applications"), participated in interdisciplinary work with researchers of other departments and laboratories. Moreover, two teachers of this group are researchers in Applied Mathematics.

From these comments and results, it is obvious that real applications produce positive reactions in engineering students, in concordance with experts’ opinions [12-14].

6. Conclusions

As it was mentioned in the previous section, an expert group was consulted about mathematics teaching and learning at the undergraduate level, focusing in the specific case of engineering careers [14]. Most remarked the importance of teaching significant concepts and procedures in service courses. On the other hand, chemistry and engineering students showed an important preference for teachers who make the effort of presenting real-life problems, related with their own careers [12-14].

When students of differential equations were consulted about these courses, there were positive reactions, when motivating examples are used to promote mathematical modelling and applications. Moreover, they enjoyed working together in project-work, trying to propose mathematical models and/or applying the different concepts, tools and techniques to solve them analytically or numerically [15].
The need for relevance was highlighted by many writers as being important in assisting students with learning mathematics. For example, Bajpai et al. [16] suggested a range of improvements including a modelling approach and providing more relevant examples. According to Wood et al. [17] ‘To make a mathematics course seem relevant to engineering students – and hence worth an investment of time – the subject has to be made to seem valuable for their own specialization and future cases’.

Finally, Mc Alevey and Sullivan [18], asserted that there is a need for using real-life problems since, ‘Students are best motivated by exposure to real applications, problems, cases and projects’.

Motivation is not the unique reason for introducing modelling and problem solving activities in engineering courses. For instance, it is possible to present a sophisticated mathematical tool or concept in a preliminary version, immersed in a motivating context, through real-life problems. To achieve this goal, these concepts and tools must be in the Zone of Proximal Development of the students [19], so, if the problem has a high degree of difficulty, it usually needs a Didactic Transposition [20], in order to convert the original problem in a suitable version for second year university students. This is exactly the situation in several chemical kinetics problems, while mixing problems can be introduced almost in their original versions, at least in differential equations courses, usually placed in the fourth semester (i.e., at the end of the second year). For this reason, mixing problems are used to illustrate several procedures, which are very common when operating with O.D.E. linear systems, such as diagonalization, changes of variables, etc.

Another important reason for including modelling, inverse modelling and problem solving is to expose the engineering students to other processes which are almost absent in other courses without these modelling and problem solving activities. In fact, as Cavallaro et al. mentioned “it is also important for an engineer’s professional performance to make decisions and to make correct estimations. These estimations do not always follow the procedural characteristics that students have met in traditional courses” [21]. Chemical kinetics and mixing problems (among others) had been successfully to introduce this kind of procedural characteristics. For example, students are asked to estimate a priori the qualitative behaviour of a salt solution in a tank system and/or they are asked to predict which can be the internal geometry to get a desired result at the output. These estimations are compared with the final results and if there are differences between both (their a priori estimations and the a posteriori results), they are discussed in class. The following sequence: 1.- A priori estimation of the salt solution behaviour; 2.- Modelling or inverse modelling; 3.- Solve the O.D.E. linear system and 4.- Comparison with the a posteriori results; cannot be usually find in traditional courses.

Another aspect that must not be ignored is the type of assessment must reflect the teaching method of the topic. The evaluation process must not be dissociated from the style of teaching. So, if courses are have been instructed through problem-solving, modelling, etc., then assessment must be carried out to reflect this. This purpose can be put into practice through project-work, where students –with orientation of an interdisciplinary team of teachers and lecturers– try to solve real problems of their careers, in order to approve their mathematical courses [15]. Mixing and chemical kinetics problems are excellent sources for this purpose. 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.
According to Blum and Niss in their classic paper about applications, modelling and applied problem solving [22], there are six different types of basic approaches to including relations to applicational areas in mathematics programmes. In our course, at the beginning (1966 to 2000), the “islands approach” was the selected one. In this approach, the mathematics programme is divided into several segments, each organized according to a two-compartment approach: a first part of a usual course in “pure” mathematics whereas the second one deals with one or more “applied” items, utilizing mathematics established in the first part or earlier. Gradually, the course changed to a “mixing approach”, where elements of applications and modelling are invoked to assist the introduction of mathematical concepts and conversely, newly developed mathematical concepts, methods and results are activated towards applications and modelling situations whenever possible.

Finally, as it was suggested in the foreword of iJMEST special issue, devoted to Calafate Delta ’07 Proceedings, ‘Current students are presented with an enormous range of choices of courses and career pathways. In this competitive environment, the biggest challenge for mathematics departments around the world is to attract students to mathematics’ [23]. In order to attract these students, it is important to note that for most engineering students, intrinsic motivation appears when it is felt that they are solving problems in which they have an interest. For example, Smith and Wood [24], said “we feel that this is an effective way of introducing mathematical concepts to engineering students, whose main interest in mathematics is often limited to its usefulness in their future profession”. In the same direction, Brown et al. [25], argued that meaningful learning will only take place if it is embedded in the social and physical context within which it will be used, and if it involves what they call ‘authentic activity’ or ‘ordinary practices of the culture’.

Searching for new real-life problems to be used in mathematical courses for engineering students, represents an interesting challenge for engineers, mathematicians and mathematical education researchers and, at the same time, it provides a good opportunity for interdisciplinary work in both research and teaching.

7. References


