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The Pedagogical Implications of Using MATLAB in Integrated Chemistry and Mathematics Courses*

LARS ÖHRSTRÖM, GÖRAN SVENSSON, STIG LARSSON, MICHAEL CHRISTIE and CLAES NIKLASSON
Chalmers Tekniska Högskola, SE-412 96 Göteborg, sweden. e-mail: ohrstrom@chalmers.se

The last years the undergraduate chemistry and mathematics courses at Chalmers Tekniska Högskola (Chalmers University of Technology, Sweden) has undergone a major curriculum reform. One of the driving motives behind the reform was that students should learn to use mathematics as a real tool for solving chemical problems. Mathematicians and chemists, with pedagogical help from an educational expert, changed the traditional course structure in terms of organization, content, and teaching and learning methods. This paper concentrates on the use of MATLAB in laboratory work and in individual and group assignments. It deals, in particular, with the pedagogical benefits that the designers of the new course saw in presenting real chemical problems that could be solved using applied mathematics and the MATLAB software. Student experience was evaluated both by the teachers and the educational consultant and responses are largely positive. Increased student learning can be seen through higher motivation and synergy effects of treating chemical problems in the MATLAB tutorials. The most serious problem is to give all students the necessary MATLAB skills and a risk is an overestimation of the MATLAB proficiency in subsequent courses leading to disproportional workloads on projects and little time for reading and study.

INTRODUCTION

A SOMEWHAT PROVOCATIVE definition of the difference between engineering and academic research is that while in academia we solve problems that *can be solved*, engineering deals with problems that *have to be solved*.

In engineering education this is traditionally mirrored by the focus on analytical solutions during the first years, and 'real engineering problems' of the final years. In the first case, emphasis is on the understanding of mathematical, chemical and physical phenomena by the treatment of cases solvable by analytical methods. In the second case, more weight is put on obtaining numbers that are solutions to engineering problems via more or less 'black box' computer programs. In the intervening time the students have normally encountered courses in numerical analysis, computer programming or applied mathematics to prepare them for this situation.

This division between the solution of special cases (i.e., analytic integrals, hydrogen atom wave-functions, equilibrium problems reduced to two variables) in both mathematics and chemistry, and the often unrelated treatment of 'unsolvable' equations in numerical analysis, causes problems in chemical engineering courses. Teachers often do not know which leg to stand on but feel instinctively that today's engineers need to balance on both practical and theoretical 'legs'.

Chalmers Tekniska Högskola (Chalmers University of Technology, www.chalmers.se), located in Gothenburg on the west coast of Sweden, is one of the country's two 'old' engineering schools. It has over 8500 M.Sc. and B.Sc. students (25% women), more than 1000 PhD students (26% women) and 2450 employees. The school is a major supplier of technical and scientific personnel as well as, middle and high-level management for the Swedish industry. There are 13 different national 4.5-years (230 ECTU) MSc programs divided among separate schools of, for example, electrical engineering, engineering physics and chemical and biological engineering. The schools have different curricula but there is a degree of coherence in content and structure. Usually the first three years consist of compulsory courses and the last 1.5 years comprise elective courses and diploma work. In the first year, mathematics and natural sciences dominate the course selection. The second year is more applied, still with considerable amounts of mathematics and computer science. In the third year, the applied engineering courses dominate and very little mathematics is taught.

In the School of Chemical and Biological Engineering at Chalmers we have advocated an integrated approach between mathematics and chemistry as a remedy to this problem [1, 2]. MATLAB and its use in solving real problems in

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mathematics and chemistry already in the first semesters is an essential part of this strategy.

SHORT PRESENTATION OF THE COURSES AND STUDENTS

The courses in question are one in mathematics (22.5 ECTS) and one in general chemistry (21 ECTS) making up 95% of the first-one-and-half semester of the three-master programs: Chemical Engineering, Chemical Engineering with Physics, and Bioengineering. (ECTS = European Credit Transfer System; in the Swedish setting 3 ECTS represent 2 weeks of full-time studies, exams excluded.)

As textbook in mathematics we use a new book [3] written especially for this approach to teaching and learning mathematics at a technical university. In the chemistry course we use three books [4–6]. This course program was given for the third time in the academic year 2004–2005. The total number of first-year students in these programs is 180.

The students belong to the upper half of the Swedish secondary school graduates with grades that are high or above average. Most are 20 years or younger when they start their university studies, and come directly from secondary school, but a fairly large minority (11%) are 23 years or over and some have been admitted in other quota groups. (The Swedish system with different quota groups enables also older students with different backgrounds to be admitted to higher education.) Key problems are the varied backgrounds, ambitions and abilities of our students, how not to bore the best, well prepared students while still caring for the other end of the spectrum.

The reformed chemistry course takes a unified approach to chemistry. It combines material from old courses (in inorganic, physical, bio, and organic chemistry) in a way that stresses common themes and paradigms in contemporary chemistry, in contrast to the emphasis on the differences, and the consequential fragmentation and compartmentalization, of the old curriculum. Details, philosophy and practical aspects of this new chemistry course will be described in a separate article.

INTEGRATION OF THE COURSES IN MATHEMATICS AND CHEMISTRY

Mathematics is a fundamental subject in engineering and our goal will never be a 'mathematics for chemists' toolbox-based course. However, both subjects can benefit from interactions and exchange of examples. In fact, for most mathematical concepts introduced there is an appropriate chemical problem that can be solved. The challenge is to make all teachers aware of this and then use it to increase the learning of the students.

We have had continuous discussions between our teachers in chemistry and mathematics since 1998, and without this the project would have been impossible. The integration is manifested in many ways in the two courses: exchange of teachers and course material, schedules and planning, identifying topics where it is appropriate to work together, but most important is a number of MATLAB-related projects and exercises. Most of these give credit in both courses, and they are compulsory assignments.

MATLAB EXERCISES AND PROJECTS

We will now give a short description of the different MATLAB assignments. It should be noted that the students do not use the toolboxes available in MATLAB. As part of their mathematical training they write their own subprograms.

The general idea behind these projects is that the mathematical concepts and skills should be learned and developed in the mathematics lectures and tutorials. Appropriate MATLAB programs should then also be prepared. Then the students are introduced to a chemical problem where these skills are needed. The chemical problem should then be formulated in a way that makes it solvable by the mathematical tools developed. During this second part teachers from both disciplines are present together in the computer studios.

Introduction of the 3d geometry of molecules and mathematics

In this 4h computer laboratory exercise the students make models of ethane, (CH_3CH_3) and ethene (ethylene, CH_2CH_2) using MATLAB. Specifically, they rotate the CH_3 and CH_2 groups and use electrostatic repulsion potentials to derive the most stable geometry. In this way matrix transformations and cylindrical coordinates are conveniently introduced. In a second part of this exercise a commercial 'black box' quantum chemical program is used to do the same geometry optimization and the students have to contemplate the reasons for the discrepancies of these two methods of calculations when it comes to ethene.

Here it is interesting to note that most of our students know the geometry of ethene (flat torsion angle 0°) from the chemistry lecture. But, after having calculated the geometry using MATLAB, they could very well think that the hydrogen atoms are oriented perpendicularly (torsion angle 90°). This illustrates one ambition with these projects, to stimulate the students to use their chemical skills when working with mathematical problems and *vice versa*.

Differential equations and kinetics

This project is an independent individual assignment where the students work on their own, but there is also designated time in computer studios with both mathematics and chemistry teachers. The task given to the students is to model a multi-step chemical reaction, for example the CFC (chloro-fluoro-carbons) + ozone system.

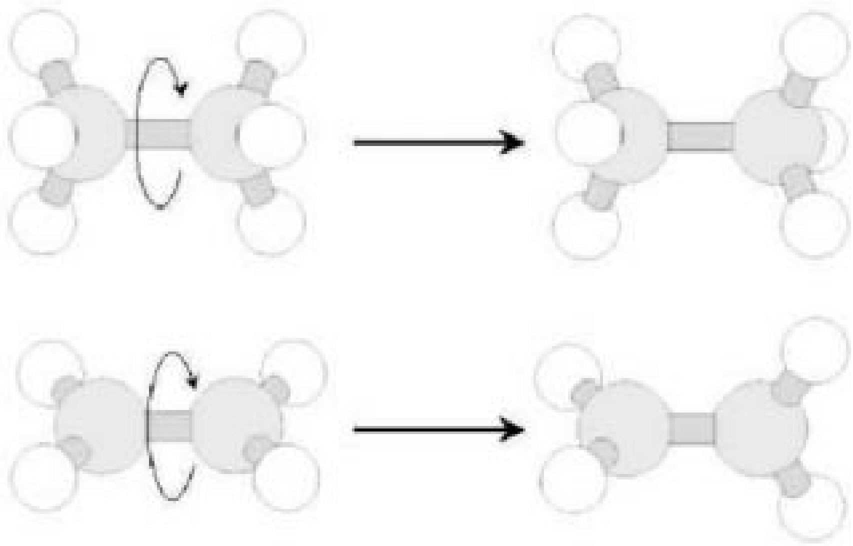

Fig. 1. Three-dimensional geometry, matrix transformations and cylindrical coordinates introduced by models of ethane and ethene in MATLAB.

They have to write the separate differential equations corresponding to each chemical reaction and then couple them using a self-written MATLAB program for solving ordinary differential equations. The final outcome is a graph showing the concentrations of each participating species as a function of time. Each assignment has a number of supplementary questions, encouraging the ambitious students to explore the system further. A full traditional project report is submitted by each student.

Systems of nonlinear equations and equilibrium analysis

During the mathematics course the students write their own MATLAB program for the solution of systems of nonlinear algebraic equations by Newton's method. During one of the scheduled studio tutorials they pick one environmentally related equilibrium analysis problem. This should be completed and checked off by any of the present mathematics and chemistry teachers before leaving. In a traditional setting the students stumble as much on the mathematical difficulties as the chemistry.

Now, in principle, they can concentrate on building the chemical model and the equations, while the solution is taken care of by their pre-written MATLAB program.

Computer laboratory on acids and bases

In this laboratory exercise the students treat data from the titration of an amino acid with a

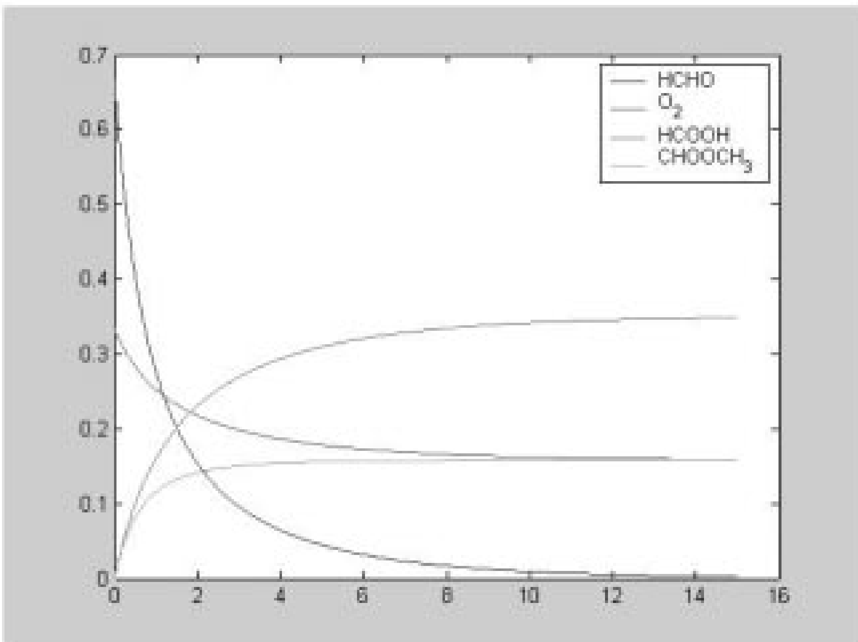

Fig. 2. MATLAB simulation, using chemical reaction kinetics, of the oxidation of formic aldehyde.

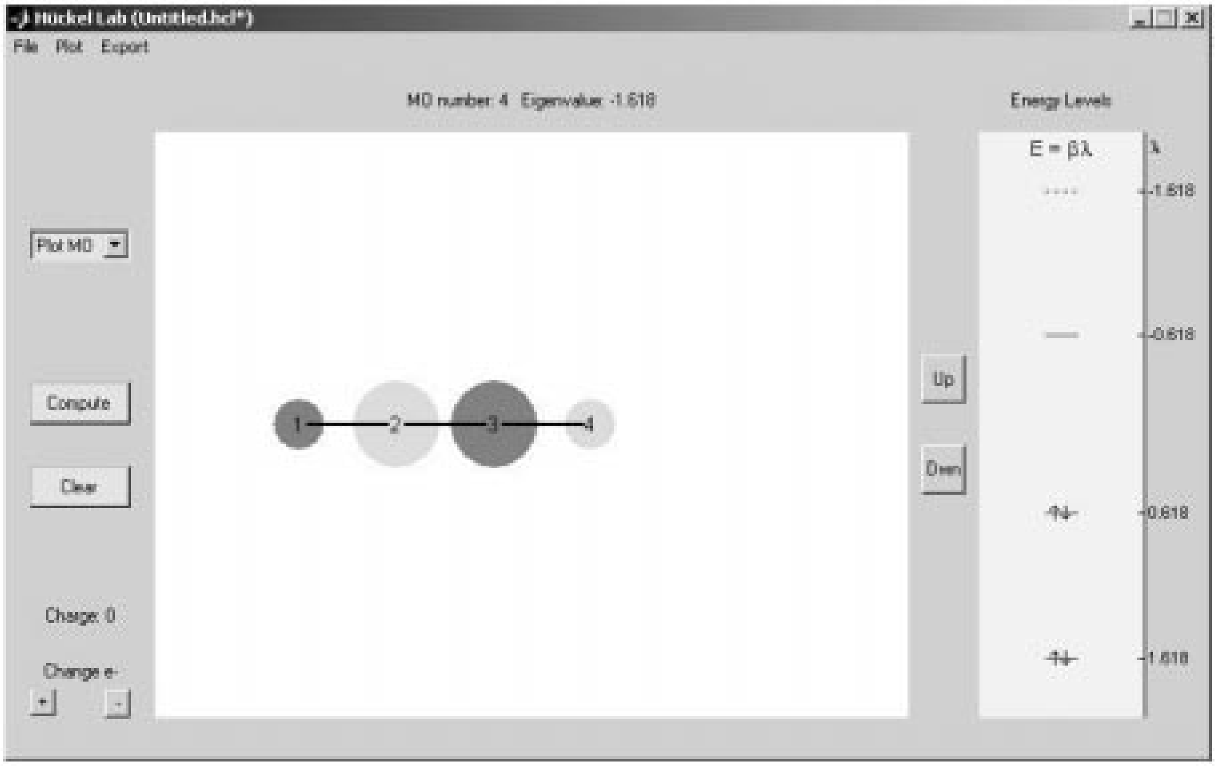

Fig. 3. Chemical input (butadiene molecule) to the program HuckelLab[7] written in MATLAB. The student draws the configuration of the molecule, the program then computes its Hückel matrix, the corresponding energy levels and orbitals (eigenvalues and eigenvectors) and displays them in the diagrams. The data can be exported for further computations in MATLAB and in the chemistry laboratory. This program is also used in other courses.

strong base. The derivative dpH/dV should be constructed from the given pH = f(V) data using MATLAB or Excel. Although mathematically not very demanding, it provides a practical example of the use of mathematical computation in analytical chemistry. (Other such assignments valuable for analytical chemistry is equilibrium analysis and kinetics.) From the resulting plot the acid constants of the amino acid can be calculated and compared to data from the literature.

Computer-corrected test in equilibrium analysis

As the end point in the course segment treating acids and bases, and solution chemistry, the students are given a computer-corrected test. Most problems are easily solved using a hand calculator, but the final question is of the same type as in the studio assignment on nonlinear equation systems, and they are encouraged to use MATLAB to solve this.

The eigenvalue problem and molecular orbitals

A matrix eigenvalue problem connected with molecular orbitals (the Hückel method) is introduced by mathematics and chemistry teachers during a shared lecture. Subsequently a studio tutorial is scheduled where the students do a few selected calculations by hand and then move over to a Hückel program [7] written in MATLAB for some more elaborate calculations. The results should be checked by any of the present mathematics and chemistry teachers before leaving, and data stored for use in a later laboratory exercise. During this later practical session in the laboratory, the students extract lycopene and β-carotene from tomatoes and carrots and measure the absorption maxima and compare this to the calculated value.

EVALUATION

In order to investigate how well the new courses work, but also how the changes have been accepted, several forms of evaluation [8] were carried out. We will briefly present the results here:

1. **Formative evaluation during the course.** Described in some detail above. As can be expected from the varied background of our students we see all kinds of results, from very good to terrible. Despite the efforts at the very start of the courses, programming is clearly still a weak point for many students, and many find MATLAB difficult.
2. **Interviews with second-year teachers.** 'Fundamental and engineering thermodynamics' is a second year course that also uses a lot of MATLAB programming and that relies heavily on the first chemistry and mathematics courses. Interviews with the two principal teachers confirm that some students still lack essential MATLAB skills. They suggest that the major

improvement needed is programming skills and specifically how to debug programs.

3. **Evaluation by independent experts.** During and after the first year of the new curriculum the courses where evaluated by an independent group led by a pedagogical consultant. The team used questionnaires and interviews with teachers and students. They found that the students appreciate the idea of higher integration of mathematics in chemistry. However, to work in practice such integration needs to be developed further. The main point for improvement was communication between teachers in mathematics and chemistry. For example, it is essential that all involved teachers (about 40) give the same answers as to what are the formal requirements of each assignment and report.
4. **Independent evaluation by the students.** Every year the students performed their own independent evaluation of the courses based on a handout questionnaire. Points raised here were the difficulties or high levels of some projects, lack of time, and again communication between teachers. Some students seem to demand that *all* teachers know *everything* about chemistry, mathematics and MATLAB, which is clearly unreasonable.
5. **Evaluation by the students on the courses website.** After the final exam the students from both years could contribute their opinions on a website questionnaire. For each part in the course, plenary lectures; projects; and the integration between the two subjects etc., the students were asked two questions: (1) what was good and (2) what was bad. Some of the comments that students volunteered on the survey the first year were 'Great idea to combine mathematics and chemistry', 'It's good to see that what one learns in mathematics can actually be used in chemistry', 'Excellent to have applications' and 'Some of the mathematics-chemistry projects were really good. It was good to see why mathematics is important and that early in one's education learn to apply one's knowledge'. Some negative comments were 'Did not work very well, mostly because there was no teacher who could answer questions on both chemistry and MATLAB', 'Did actually not see much of this integration', 'Cannot see if I really benefited from this'.

In the second year, efforts were made to address the problems found after the evaluations of the first year. This clearly led to an improvement, as can be seen Fig. 4.

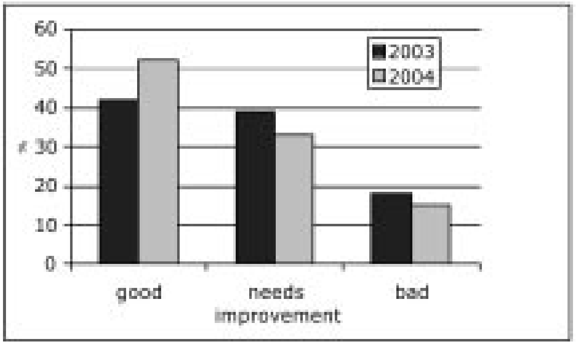

Fig. 4. Student opinions on the mathematics/chemistry integration submitted to the website questionnaire. The number of answers to this question rose from 33 in 2003 to 43 in 2004. In 2004 the total number of students answering the survey was around 30%.

DISCUSSION

The evaluations raise several questions in many categories and we will begin with issues close to the students and finishing with concerns relating to management and administration.

Integration

In order to be successful, an integrated approach between two subjects has to demonstrate the benefit to the students. Areas must be found where it is obvious that both sides take an interest, but where it is also clear that they are dependent on each other.

We see two fundamentally different uses of mathematics in a chemical engineering program. The first is what is usually encountered during the first years: mathematical tools are used to derive and prove many theorems and equations in chemistry. The reason is not only to give relations that can be used to calculate answers to problems, but also to provide understanding—why the equations are correct.

While this is important, and implies that students should still know how to integrate dx/x and similar expressions by heart, another use of mathematics is important in an integrated curriculum: the calculation of practically important quantities from equations without analytical solutions.

The student does not usually encounter this until the chemical engineering courses in the third and fourth year, and may thus have been under the false impression that most problems have analytical solutions, or solutions obtainable only through clever approximations. To master this type of problem, a deeper understanding of the chemical systems is often required, in addition to the mathematical know-how, and this is still an important goal. Also the so-called 'Fermi solutions' [9], the quick calculation of an approximate answer to almost any problem, can never be replaced by computational number-crunching. It is thus very important to strike the right balance between computational methods and traditional analytical methods.

The problems on nonlinear equation systems and equilibrium analysis demonstrate this well. During the exam many students show that they can do correct mathematical model building of the systems in question. However, they lack the experience to find the one clever model that will lead to

$$\begin{cases} ab^2 = 10^{-4.8} \\ \dfrac{c}{ab^2} = 100 \\ b - 2a = 0.95 \end{cases} \quad \begin{cases} (0.025 - c - y)b^2 = 10^{-4.8} \\ \dfrac{c}{(0.025 - c - y)b^2} = 100 \\ b + 2c + 2y = 1 \end{cases}$$

Fig. 5. Two equally valid chemical models for the system Pb^{2+}/$PbCl_2$(s)/$PbCl_2$(aq)/Cl^- with given initial concentrations resulting in two different equation systems related by variable substitution. The first two equations are equilibrium constants and the last is a mass balance. Both systems are easily solved by the approximation $a = 0$ or $c + y = 0.025$ in the last equation, but the first set will be much easier to work by hand. In MATLAB on the other hand the differences will be very small.

equation systems that are easy to solve by hand, see Fig. 5. Thus in a traditional exam setting they will fail the problem and feel frustrated, while with MATLAB obtaining a solution is more independent of the model chosen.

Morover, the importance of numerical calculations, also for the more fundamental mathematical education, has been stressed [10, 11]. The interaction medium between mathematics and chemistry will be a suitable programming language. We choose MATLAB, for the following reasons: availability, flexibility, generality, engineering usefulness, stability and simplicity to use and learn. It can be used on several levels, from a simple calculator to a rather advanced programming language with powerful tools for graphics. On the advanced level it also contains many 'toolboxes' for various fields of engineering [12].

There are, however, problems with this approach. MATLAB is expensive. Previously we had a 'site licence' for students and faculty but the costs became too high and the number of licences is now limited, complicating the administration. By focusing on MATLAB as the only tool we have risk of creating a mono-culture. The old curriculum contained a separate computer course using a standard programming language. This is now integrated in the mathematics course and the students are expected to get their programming skills from writing their own code in MATLAB.

We, however, believe that the benefits of using one common tool in chemistry and mathematics are far more important than the drawbacks. The choice of MATLAB may be changed if the cost gets too high, but we will then choose a common tool again, which both chemistry and mathematics can use.

Student reactions

It is obvious from the surveys that most students support the integrated approach. It is also clear that a minority dislikes it. From discussions with students, and examination of the evaluations, three different reasons for this emerge.

The first is founded in a conservative view, a certain feeling that you get cheated when the courses are (or are imagined as) not as difficult as they used to be. To some extent this view is reasonable. Completely separate courses, often with different nomenclature, force the students to find and work out the integration by themselves and this probably leads to a deeper level of understanding than an integrated approach. However, from the experience of third and fourth-year teachers, few students nowadays manage this on their own. Logically, some of the most ambitious students take this view.

The second group is on the other hand found among those students that, for different reasons, have weaker results. This is also fairly logical, since student groups that earlier had difficulties with both mathematics and chemistry courses and frequently postponed one of them (usually mathematics) are now forced to do, and be reasonably successful in, both subjects at the same time. On the other hand, it can be argued from the surveys that a fair number of students in this group are helped and motivated by this approach.

A third group of discontented students are those who have developed an animosity towards MATLAB. They may like the integrated approach, but they do not like to work with MATLAB. Student views are clear about the remedies: they want more explicit tutorials on MATLAB and more teachers helping them. However, this may not be the final answer (apart from being forbidding because of financial restrictions) since the problem could partly have another origin.

The mathematics course is advertised just as a mathematics course; you obtain formal credit for mathematics, and MATLAB is just a tool to get there. The assessment of programming and computer science is implicit and never spelled out to the students. These are skills that they are expected to acquire during the course, and most students do so. However, during tutorials and 'online' assessment they are almost never alone with a computer, and there is a good chance to hide behind a fellow student. Although the school provides good computer facilities to train on your own, and student MATLAB licences are available at a low price, some students do not see MATLAB as an essential tool, and something that they have a certain responsibility to learn by themselves right from the start, and they frequently encounter problems as the courses advance.

Thus, the conclusion is: make the MATLAB and programming tutorials more explicit, and send a clearer message to the students in terms of formal examination of programming knowledge, or maybe even change the name of the mathematics course.

Student learning

Unfortunately, positive student reactions do not necessarily correlate with increased student learning. However, we do see more motivated students, and this should in general mean that they work harder and learn more.

Another thing is the synergy effect obtained when chemical problems are treated in the mathematics course. We note several cases when students claim to have learnt kinetics or equilibrium through the MATLAB tutorials (or even from mathematics teachers!).

Formal assessment, however, does not give many clues. This is due both to the complete reshuffle of the curriculum, making no exams equivalent to any of the old ones, and to changes in the secondary school curricula, making the 'new' and 'old' students difficult to compare.

A danger is that MATLAB skills may be overestimated in subsequent courses, with the consequences that students spend too much time on project assignments, because of technical difficulties, and less time reading and reflecting on the course material.

In the following years of the curriculum one of the goals were to change the emphasis in Chemical Engineering subjects from analytical solutions by dribbling with mathematics, to focussing on problem formulation, and interpretation of the results. Parameter sensitivity, model building, prediction and discrimination are issues that are best exposed in computer simulations. Many new projects and assignments have been developed to take advantage of the new facilities and learning strategies. So far it seems to be successful. Focus must now be on how to continuously use MATLAB through the whole curriculum and in every (suitable) course except where commercial 'black-box' programs are more appropriate.

Teacher reactions

The reactions from the chemistry and chemical engineering faculty have generally been positive. Discussions reveal two important reasons: either one remembers mathematics courses filled with meaningless proofs learnt by heart and theories never applied, and thus embraces a course that actually tells the student what all this is good for, or one recalls with some pleasure the mathematics learnt but realizes how much more fun it would have been to study it in the new way.

In the mathematics department our approach is somewhat controversial and not universally accepted. The new mathematics courses were developed by a group of teachers with a background in research in computational and applied mathematics, and this is strongly reflected in the courses. With this background, the idea of using numerical computation and engineering applications as a means of reforming the teaching of mathematics is more natural than it is for our colleagues working in 'pure mathematics'. There is also a misconception that our approach is entirely computational and that we have discarded all analytical methods. However, using computers in mathematics courses is not controversial, and almost all undergraduate mathematics courses at Chalmers include MATLAB exercises to some extent, but these are usually added without changing the rest of the courses.

For the chemistry teachers involved in the course, from the former departments of inorganic, organic, physical, polymer, and nuclear chemistry, the starting points were very different. Some had used MATLAB in their research, some had encountered it occasionally, and others had followed an introductory course given by the mathematics teachers. Yet others had had no contact with either MATLAB or mathematics beyond arithmetic since their undergraduate studies. Their overall reaction was positive, although there is some frustration caused by the inability to sort out all possible problems for a particular student's assignment. This, however, is a consequence of the integration, and something we have to accept. More important is the lack of communication experienced in some cases, both between mathematics and chemistry, and between chemistry teachers

The chemistry teachers are all located in the same building which means that they meet spontaneously in the corridors, in the café, etc. This is a big advantage for the communications between them. Unfortunately such an easy interaction is not possible with the mathematics teachers since they are in another building. This naturally means less spontaneous interactions, which must be compensated for by regular formal meetings.

Management considerations

Communication problems can normally be traced to management failures. We have, on the chemistry side, introduced the concept of teaching teams, implying a very democratic management of the courses. However, with many persons involved it becomes cumbersome to take all decisions collectively. Possibly, this was a necessity during start-up, and when the courses are well defined and established the principal teachers can make more decisions on their own.

A student-related management problem arises because of the large number of independent mandatory assignments, about 20% of these using MATLAB. We use an in-house developed Learning Management System (LMS) based on FileMaker [13], both in order for the teachers to keep track of the students, but also in order to clearly show the student what the requirements are and if any assignment is missing. This system has met with universal acclaim from both teachers and students.

While not a key issue in this article, we also have to keep in mind the hard strain most university teachers are under by the demands from university management of increased performance and happier students at a much lower cost than before. Major curriculum development under such circumstances must have strong moral backing from local management, and without the continuous support from many years of different deans and boards at the School of Chemical and Biological Engineering the development described in this article would not have been possible.

Curriculum considerations

First we note that the implementation of a mathematics and MATLAB integration with chemistry would have been very hard in the traditional setting of many small chemistry courses.

Secondly, an important task is to take this project further to the second, third and fourth year. That is, the MATLAB and modelling skills developed (and whatever sacrifices made in other areas) have to be mirrored in the curriculum of the following years. This implies strong vertical interactions, going far beyond sitting in committees and discussing course names. We believe we are on the right track, with the closer contact generated in the last years between teachers of chemistry, mathematics and chemical engineering. We therefore view with some alarm efforts by larger institutes of technology and universities to 'sell out' the first years of the M.Eng. education to smaller university colleges and retain only the final years [14]. One of the important differences between an engineering school and a university should be the carefully 'engineered' curriculum with a clear purpose of the former, and the freer and more curiosity related curriculum of the later. Both systems fill valid needs in a modern society.

CONCLUSIONS

MATLAB was chosen as the medium through which a successful integration of mathematics and chemistry in the first year of our M.Eng. programs could be built. Mathematical skills were translated to MATLAB programs by the students in order to solve real chemical problems. Thus, mathematical model building was introduced early in the curriculum.

Student and teacher responses are largely positive. Increased student learning can be seen through higher motivation and synergy effects of treating chemical problems in the MATLAB tutorials.

The most serious problem is our failure to give all students the necessary MATLAB skills. We believe one remedy is to also in a formal way stress the programming and MATLAB skills in the mathematics course, maybe even to such an extent as to change the name of the course.

One risk is an overestimation of the MATLAB skills in subsequent courses leading to disproportional workload on projects and little time for reading and study. Related to this is the risk that advances made in the first years are not profited on in later years, due to either bad vertical communication or deliberate decisions by higher management to geographically or administratively separate the early (basic) years in the engineering education from the later (applied) years.

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Lars Öhrström is professor of Inorganic Chemistry at Chalmers University of Technology, Göteborg, Sweden. He is coordinator of the first year integrated chemistry course for the three engineering programs at the department of Chemical and Biological Engineering. He obtained his M.Sc. and Ph.D. degrees from the Royal Institute of Technology in Stockholm. He did post-doctoral work on molecular based magnetic materials at the Commissariat à l'Energie Atomique in Grenoble, France, 1993–1995, and in 1995 he returned to Sweden and started his work at Chalmers. He became a senior lecturer in 1997 and professor in 2004. His main research interests are experimental and theoretical approaches to molecular based materials and crystal engineering with focus on coordination compounds and three-dimensional nets.

Göran Svensson is currently an Associate Professor in Inorganic Chemistry at the Chalmers University of Technology. He is working in the area of solid state chemistry, and is primarily interested in oxide materials with optical properties. The main goal is improved materials for applications such as detectors and wave-guides. In this work the establishment of structure-property relations is important. At present he is also working as the CIO (Chief Information Officer) of Chalmers. As CIO he is responsible for the development and use of information technology at the University. He is also involved in teaching where he is responsible for the advanced course in Solid State Chemistry. He has M.Sc. and a Ph.D. degrees from Lund University, Sweden.

Stig Larsson is an associate professor of Mathematics at Chalmers University of Technology, Göteborg, Sweden. He is the coordinator of a reformed mathematics course in three engineering programs of the School of Chemical and Biological Engineering. He got an M.Sc. in Engineering Physics in 1976 and a Ph.D. in mathematics in 1985 from Chalmers University of Technology. After spending two years at the University of Michigan he returned to Chalmers University in 1987 as a senior lecturer in mathematics. In 1992 he became an associate professor of mathematics. His research is mainly concerned with numerical approximation of partial differential equations, with special emphasis of the mathematical theory of the finite element method. He is the author of a textbook on partial differential equations with numerical methods.

Michael F Christie is a Senior Lecturer in Educational Development and Pedagogy at The Centre for Digital Media and Higher Education at Chalmers University of Technology, Göteborg, Sweden. He was the pedagogic expert and consultant in the integration project. He is also a member of the board concerning the strategic effort on learning and teaching at Chalmers. He has a Ph.D. and BA (First Class honours) degrees from Monash University, Australia.

Claes Niklasson is professor of Chemical Reaction Engineering at Chalmers University of Technology, Göteborg, Sweden and Head of the Department of Chemical Engineering and Environmental Science. He is also responsible for graduate programs at the School of Chemical and Biological Engineering. His research interests are in the bioprocess engineering field.