Why and how can mathematics improve the learning in chemistry and chemical engineering?

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Why and How Can Mathematics Improve the Learning in Chemistry and Chemical Engineering?

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ABSTRACT

Mathematics that is taught at all engineering universities in Sweden and other countries has not been changed for a very long time. With the shift toward greater use of mathematical numerical tools in many engineering subjects, the content and manner of teaching in mathematics are undergoing profound changes. Since the mathematics often is taught early in a curriculum, it is of interest to investigate how the learning in mathematics will have an effect on the learning in chemistry and chemical engineering subjects. In the present work we discuss how changes in mathematics education might influence the way of teaching and learning for the following subjects in the chemical engineering programme at Chalmers. Furthermore, some thoughts are provided on how the changed mathematical knowledge and skills among students and also integration in the engineering subjects might affect and help in a deeper learning approach in particular chemical engineering subjects, such as fundamental chemistry, chemical reaction engineering and bioprocess engineering which are important subjects within the different Programs at the school of chemical engineering.

Keywords: Applied, Mathematics, Chemistry, Chemical, Engineering, Numerical, Education, and Pedagogic.

INTRODUCTION

Chalmers (www.chalmers.se) is a technical university on the West Coast of Sweden with over 8000 (23 % women) master and bachelor students, about 1200 PhD students (23 % women) and about 2300 employees. At Chalmers there are also 10 different national Master of Science programs, which require 4.5 years (180 credits) for a M.Sc. degree and 12 International Master programs (60 credits). The separate schools involve for example mechanical, computer, electrical, civil and chemical engineering and engineering physics and architecture. The schools have different curriculum for their education but some coherence can bee seen from their individual curricula. Usually (and this is somewhat changing) the first three years consists of compulsory courses and the last 1.5 year comprise elective courses and a diploma work (half-year). In the first year mathematics and natural sciences dominate the course selection. The second year is more applied, still with much mathematics and computer science. In the third year the applied engineering courses dominates and actually very little mathematics is taught then.

The mathematics that has been taught for many years is generally traditional, with a focus on analytical solutions to problems, in many universities. Applied courses and their problem-solving training are of course then adapted to the students' abilities gained in mathematics. The use of computers in mathematics does not match the needs as a whole. Computer use and programming are usually covered by special courses such as those on programming and within the subject numerical analysis.

At the moment there is a project going on to make changes in the way the mathematics is taught (and learned) and applied in the coming subjects in the second and third years of the master program. This learning project is strongly supported by Chalmers University of Technology (and be it noted, the students) currently concerns two separate educations named Chemical Engineering with Physics and Bioengineering. The number of students taken for these educations is 35 and 70 annually. This is a suitable small group for a development project of this kind. The new mathematics is also introduced to the chemical engineering students in the fall of 2001. In this paper the implications of this change in mathematics teaching on applied subjects for the two educations will be discussed including their advantages and possible drawbacks.

BIOENGINEERING EDUCATION

The biotechnology education is a new education, which started in 1996 with 70 students taken in annually. The number of applicants for this education has been very high, about 2.7 students for every position. In other words, it is the top students that will start this education and this imposes many requirements for a good and well-planned curriculum. In 2000 the first students from this education graduated and applied for positions in industry, research centres and universities. The related curriculum (which is under development) is shown in figure 1. For the last year a number of directions are possible such as medical and molecular biology, food science, forest and environmental science and the more traditional bioprocess engineering sciences.

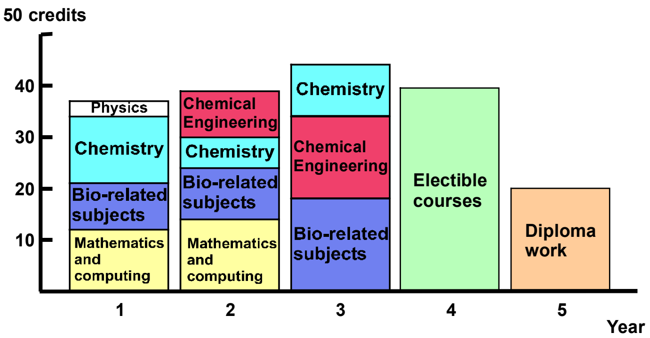
The goals for these student educations are

Identify and solve biotechnological problems
Carry out and analyse experimental investigations
Design large-scale biotechnological processes
Manage both engineering language and the language of biology

The means for achieving these goals are

Computer skill
Good knowledge of Biochemistry, Physical chemistry, and Molecular biology
Chemical engineering competence
Sufficient insight into Biology, Organic chemistry and Inorganic chemistry
An open and creative academic environment

Master Program in Bioengineering (180 credits)



MATHEMATICS LEARNING APPROACH

(http://www.md.chalmers.se/Centres/Phi/Education/KfKb)
Virtual reality and computer based simulations brings new and useful tools to science and technology. New systems' configuration and products can be designed and developed and in the later stage tested through computer simulations. This testing can be performed on time scales, and at costs, which are orders of magnitude smaller than using the traditional technique, for example, extensive lab-work, rules of thumb and direct calculations by hand. In the sciences of, for example, Bioengineering, Environmental- and Chemical Engineering, Chemistry, Economy and Medicine computational modelling can be applied with great success and also with the aim of getting a more fundamental and deeper understanding of the phenomena involved.

Computational Mechanics, Physics, Fluid dynamics, Electromagnetics, Chemistry, chemical engineering and Biology are all subjects, which involve the solving of systems of differential equations by using computers. Nowadays we consider reactor analysis to be the heart of a process design procedure but in the future the heart of process design might be moved into the new fields of new simulation techniques such as Computational Mathematical Modelling (CMM) and Computer Aided Design (CAD).

At present the need to modernize engineering education is very challenging; especially the new tools of calculation such as CMM/CAD will be very interesting in this context. This technology can be used to build crossings between subjects, schools and courses previously considered to be separate. The form as well as the content, from basic to graduate level, should be changed with this in mind.

Mathematics, the way that it is introduced and taught (learned) is a foundation of the applied sciences in all schools and at all levels, since engineering and science are largely based on mathematical modeling. The quality and level of mathematical learning determine the status of the total education. Modeling in the engineering subjects and education has changed towards the use and development of computers. An integrated education is therefor necessary for a successful engineering curriculum. This integration is planned and discussed in many technical universities at present. The variance and spectrum of how much and what should be changed differ, according to weather one asks mathematicians or computer scientists.

Engineering subjects often consider today's traditional mathematics to be of little use. Problem formulation and solution in these subjects has therefor been limited to analytical solutions. The topic of (and the solving of) differential equations is kept at an elementary level for this reason. Careful selection of problems and instructions is the reason for this procedure in mathematics education. The reduction in mathematics education in some schools at Chalmers can be understood from this fact. Mathematics is indeed difficult and hard to penetrate in a useful way, but in the age of computers this is not a good trend for mathematics all over the world.

The project at Chalmers deals with the synthesis of mathematics, computation and the handling of differential equations in the form a general computational methodology. This project is deeper and goes further into non-linear systems already in the first half year (compared to previous curriculum). The program involves a more constructive education with active student participation and feed back communication between student and teacher. Including of realistic and applied examples helps and motivates in this context. After the new preparation, students can penetrate deeper into problem-solving and interpretation with much less instructions and teacher interaction and guidance. The program can be seen as a synthesis between the computer (body) and mathematics (soul) with the aim of coming as close as possible to reality and its complexity.

In the fall of 1999 the new mathematics program in the Bioengineering and Chemical Engineering with Physics educations is providing a new basis for the interaction with all engineering courses in the second and third year. This is necessary in order to fully use this new type of knowledge that the students have learned.

STUDENT INTERACTIONS IN MATHEMATICS

Every week the students and teacher meet in 4-hour lectures (traditional) and in exercises of 4-6 hours in tutor groups (8 students) including problem-solving, projects, and case studies with written and oral presentation. These exercises are lead by two teachers one more experienced and one Ph.D. student (probably senior students in the future). Due to this high quotient between teacher and students in the exercises the use of older students as junior supervisors at these exercises will probably develop in the future. These exercise classes also gives the students more time to reflect and solve problems early in their mathematical training. More applied examples are brought into the education at an early stage. Material for the first courses has been developed in a compendium (which will be published in a traditional book in the near future) [1] but the book by Eriksson and co-workers [2] is also used in this learning strategy.

The applied mathematics is taught parallel to computer sciences, which means that problems are sometimes solved by the writing and use of individually student made computer programs and subroutines. The computer program for programming is MatLab but the students do not use the toolboxes available in this program. As part of their mathematical training they construct their own subprograms for this purpose.

PROJECT DESCRIPTION AND AIMS

The main goals of the project:

To implement and evaluate the benefits of integration between the new mathematics courses and the chemical engineering courses on many levels using the platform provided by the new mathematics.

To attain a deeper learning approach to chemical engineering fundamentals including realistic modelling of scientific and technical phenomena.

Increase independence in work situation for the students and more interdisciplinary assignments and projects.

Increase the possibility to introduce new and varied forms of teaching (and learning situations) in different courses.

Change the students/teachers attitude towards learning by introducing new forms and ways of assessment/examination of student learning that are designed to encourage a deeper understanding of the subject.

Increase use of applied and realistic chemical engineering examples in the mathematics courses. Use the mathematical skills in the engineering subjects in a proper way.

Means to achieve these goals are for example; Team of teachers and larger Interdisciplinary and integrated courses (Math./Chemistry/Chem.Engn.)

Since this project is very large and time consuming for the teachers (both in terms of development of new material and implementation thereof) the project has to focus on:

Do the tools come into focus instead of the basic understanding of the fundamentals?

Will the view of the students and the teacher's change concerning what is important to learn?

The view must probably be co-ordinated concerning what, when and how to learn certain things.

Will the workload of the teachers and students and how they work change drastically?

Do these pedagogic changes in the learning situation suit all types of students (gender, background, and experiences...)? How will this effect the individuals?

How can we efficiently use the new and more applied student knowledge in mathematics? How can we train, inform and prepare the teachers (and students) for this mission?

How and for what purpose must the assessment/examination procedure be changed? How will this affect and foster a deeper learning approach from the students?

One big question is then:

How do we measure a good result in terms of increased understanding/learning and capabilities?

This is very hard to answer at the moment but some ways of examine this effect is to use the teachers reflection and motivated changes in teaching and learning methods, type of contact interaction student/teachers and student/student might be indicators of a improved learning situation.

As in many pedagogic projects the process in itself is very useful when the teachers actually works (find time) with development of their own teaching and ask questions such as: What phenomena can and will be described and maybe learned in a different manner than before. Why, when and how?

Approximate timetable of the project

Academic year 2001 - 2002

Preparation of the fundamental chemistry and fundamental chemical engineering courses.

Interviews with students and teachers and probably presentation of project on some conferences.

Formation of teacher teams in the courses and integration of teachers in different and interdisciplinary courses.

Academic year 2002 - 2003

Implementation of the new mathematics into the chemical engineering courses. Introduction of the new mathematics for the chemical engineering students in the fall of 2001.

Evaluation of the existing system through interviews and questionnaires.

Discussion of new projects and assessment (including varied forms of examinations) in workshops.

Start of the new integrated General Chemistry and Mathematics course for all programs at the school.

Continued development of integration of mathematics in the chemical engineering and chemistry courses

Pedagogic evaluation of first year based on learning of fundamentals and comparison with expectations.

There are over 20 committed teachers from the different fields of mathematics, chemistry and chemical engineering and a number of student representatives involved in this project. Experts in the field of pedagogy and gender research are also actively involved.

ENGINEERING COURSES

The applied compulsory engineering courses in the second and third year of the Bioengineering curriculum are for example:

Transport phenomena
Chemical reaction engineering
Bioprocess engineering
Chemical engineering design
Experimental planning and evaluation.

As three examples of what can be achieved in these courses as a consequence of this new mathematics knowledge we consider General chemistry, Bioprocess engineering and Chemical reaction engineering.

GENERAL CHEMISTRY

It is not only the gap between mathematics and chemistry that is a problem. Also the division of chemistry courses into separate inorganic, organic, analytical and physical chemistry courses creates problems. The students have problems applying knowledge gained, and matemathical methodology used, in one subject of chemistry in another area of chemistry and also in seeing the relation between different subjects of chemistry.

An additional problem is the large span of both general motivation, skills and knowledge of the first year students. This cours has to encourage and help the weaker students and still spur and motivate the top students.

Thus, integrating inorganic, organic, analytical and physical chemistry and at the same time as focusing on how mathematics helps us understand chemistry makes sense. Some examples of how this could be done follows.

Specific pedagogical problem:
Usually the mathematical treatment of quantum chemistry is postponed to 2:nd year physical chemistry. Therefore students often find the concepts of quantum mechanics such as wave function, quantum numbers etc abstract and the treatment of this subject is, by necissity, very brief in traditional general (or inorganic) chemistry courses.
Aim:
The introduction of quantum mechanics and differential equations in *both* chemistry and mathematics. Visualisation of the wavefunction and the effect of the quantum numbers. Introduction to molecular orbitals and the concept of σ- and π-orbitals.
Methods:
Project work in groups with Matlab in studios, calculation by hand, UV-vis spectroscopy.
Improvement of student involvement and learning:
By solving a number of related problems in programming, differential equations, spectroscopy and quantum chemistry the student group will draw on the potential of all its members in different areas, thus stimulating discussions and learning.
The project work will show the connection between quantum chemistry and spectroscopy. A realistic problem is solved by chemical theory and mathematical tools newly gained by the students. The direct application of the mathematical tools in chemistry will also stimulate their interest in mathematics.

Specific pedagogical problem:
Structure, i.e. the three dimensional arrangement of objects such as atoms, molecules and electron densities, is a crucial property in chemistry and a key to most other chemical properties. However, many students have problem visualising and conceptualising in three-dimensions, in case of for example the shape of orbitals and molecular structures. As if this was not enough, we do not live in a static world, so these objects also move in three dimensions, adding to the problem.
Aim:
Visualisation of atoms, molecules, and molecular orbitals. Introduction of vector analysis and solving of (molecular structure) minimising problems. Show the use of classical mechanics and the effect of electrostatic repulsion in molecular structure determination. Introduce different tools based on different levels of approximation that can be used in molecular structure determination.
Methods:
Project tasks solved in groups. Matlab, molecular models, The molecular mechanics and semi empirical programs in the program packages Spartan and Hyperchem.

CHEMICAL REACTION ENGINEERING

The teaching has been quite traditional with laboratory exercises, lectures and calculation classes. The examinations have been traditional (problems requiring analytical solutions) for a number of years. This limitation in problem formulation has been a great disadvantage when trying to make the students to approach the subject in a deeper and more fundamental way. The new preparation makes the subject more concentrated on discussing the phenomena involved in a more quantitative and basic manner. It is also possible to add new areas within the subject such as multiphase flow in different reactor configuration. Through the use of computers (now the students are used to applying computer science and mathematics for applied subjects) the teaching situation gradually are changing from developing analytical solution by dribble with mathematics to discussion of the problem formulation, solution and result interpretation. The possibility to get the student to interact in a teaching situation more like forthcoming work situation where the answers are not always given in exact two digits emphasizes a basic understanding of the subjects. The opportunity to use computer simulation for understanding chemical engineering phenomena and to examine the sensitivity and probability of a solution will further strengthen the goals. Parameter sensitivity, model building, prediction and discrimination are other subjects that can be deeper penetrated in these simulations.

BIOPROCESS ENGINEERING

The Bioprocess engineering course involves the subjects' material and energy balances, reactor analysis mass, transfer and scale up of biological production systems. The course consists of quite traditional lectures and calculation classes, a large part being the laboratory-training course. The lab consists of the start-up (batch) and running of a continuous reactor (chemostat). This lab lasts for two weeks for each group, which means that the students are occupied for this period. The applied mathematics in this course has so far involved number of calculations where the solution has been suited for analytical solution with very little discussion and interpretation of the results. With this new background for the students in applied mathematics and computer science, the teaching can directly pass to interpretation of bioreactor analysis and design results. In this subject it is important to understand the fundamental cell-metabolism, how it works and what controls it. For this purpose, there are fairly new tools for mathematical handling of metabolic flows in cells so called MFA Metabolic Flux Analysis and MCA Metabolic Control Analysis. For more details of these techniques we recommend the book *Metabolic engineering* by Stephanopoulos et al. [3]. By use of these mathematical tools, a more fundamental understanding of the cell-metabolism can be achieved. This basic understanding of cell metabolism has so far only been demonstrated through teacher guiding and showing on computer screens. Now the student can actually work (learning by doing "wrong") and will then also experience the great advantage of using modern technology on biological systems. So far the mathematical handling of biological systems have been limited by the complexity of the systems but with this new mathematical education the new mathematical and numerical tools can be used in a more thorough way directly in the learning situation. Bioinformatics, which is the systematic handling and interpretation of large amount of biological information, is a subject that will need and gain on this change in mathematics education. There is starting a Master program in Bioinformatics at Chalmers in the year 2000 (www.md.chalmers.se/Centres/SC/bioinfomaster.html).

These courses are only three examples of how students will benefit and gain a deeper understanding and an increased interest by this new mathematics. In the near future we probably will see many new examples in the engineering field.

It is furthermore our belive that they will also *learn to make connections*, or to look for them, helping them to apply science to areas not explicitly treated in the course material.

EVALUATION AND DOCUMENTATION

Pedagogic experts will evaluate the change in educations in mathematics and the integration of mathematics in chemistry and chemical engineering.

Results of he project will be presented on WebPages, Conferences within the Chalmers Strategic Project and at International pedagogic conferences. The results will also be published in international engineering education journals.

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BIBLIOGRAPHY

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Lennart Vamling is professor in Heat and Power Technology and works parttime with pedagogic support for the teachers at the school of chemical engineering

Lars Öhrström is lecturer and deputy head of the Department of Inorganic Chemistry. He is heavily involved in the development of the new integrated general chemistry course and works parttime as pedagogic support for the teachers at the school of chemical engineering