Integration of Mathematics/Numeric Analysis with Chemistry/Chemical Engineering

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ABSTRACT

In this paper, we examine how changes in mathematics education with integration into engineering subjects influence the different teaching and learning methods for subsequent subjects in the chemical engineering programs at Chalmers. This project began in 1999 and will be completed in 2005. In the period 2001-2003, major changes were made to the first year chemistry program. These included changing from traditional lectures, labs and end-of-course, closed book exams to team teaching, teaching in smaller groups, more varied assessment and greater integration of mathematics and chemistry. Preliminary results from the evaluation of this new program are given. Furthermore, some thoughts are provided on how the changed mathematical knowledge and skills among students and integration of mathematics into the engineering subjects might assist students to develop a deeper learning approach in particular subjects in key chemical engineering programs, such as fundamental chemistry, chemical reaction engineering and bioprocess engineering.

INTRODUCTION

Chalmers (www.chalmers.se) is a technical university on the west coast of Sweden with over 8500 master and bachelor students (about 25 % women), 1050 PhD students (26 % women) and 2450 employees. At Chalmers there are also 13 different national Master of Science programs, which require 4.5 years (180 credits) for an M Sc degree and 19 International Master programs (60 credits). There are separate schools of, for example, mechanical, computer, electrical, civil and chemical engineering, engineering physics and architecture. The school for chemical engineering and bioengineering have approximately 50 % women (for bioengineering even higher) as first year students. The schools have different curricula but there is a degree of coherence in content and structure. Usually (and this is changing somewhat) the first three years consist of compulsory courses and the last 1.5 years comprise elective courses and diploma work (half-year). 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.

The mathematics that has been taught for many years in almost all universities is generally traditional, with a focus on analytical solutions to problems. Applied courses and their problem-solving training are, of course, then adapted to the students' capabilities gained in mathematics. The use of computers as dealt with in traditional mathematics courses 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.

We have begun a project at Chalmers to make changes in the way that mathematics is taught (and learned) used, integrated and applied in the subsequent engineering subjects in the second and third years of the master program. This learning project, which is strongly supported by Chalmers University of Technology (and it should be noted too, by the students), currently concerns three separate programs - Chemical Engineering, Chemical Engineering with Physics and Bioengineering. The number of students admitted to each annually is 80, 35 and 70 respectively. This is quite a large group for a development project of this kind. In this paper, the project of integration between mathematics/numerical analysis and chemistry/chemical engineering will be described and the implications of this change in mathematics teaching for important, applied and fundamental subjects for the three programs will be discussed, including the advantages and possible drawbacks. Ideas and results from this project have been presented on a number of international conferences and in engineering education journals[1-5].

INTEGRATION: A PEDAGOGICAL PERSPECTIVE

In a paper in this Journal in 2000, Everett, Imbrie and Morgan discussed[6] integrated programs and argued that the interdependence between individual courses in an integrated program goes well beyond traditional prerequisites and/or co-requisites. They described three levels (first year, second year and upper division models) in an engineering program and indicated that the principal thrust was in the area of mathematics and physics. Their arguments for integration of the curriculum were that they provide (1) better motivation of students to learn appropriately by making the interdependence of the various subjects explicit,(2) more efficient and less repetitious curricula, (3) a broader framework on which more meaningful learning can be based and (4) some continuity as many schools adopt this kind of curriculum framework.

The project reported here is focused on the integration of mathematics with chemistry and various chemical engineering courses. It acknowledges the arguments for integration cited by Everett et al but takes the pedagogical argument further.

Bowden & Marton have argued[7] that the essential role of university undergraduate education is to help students to become capable of dealing with professional situations in the future that can't be prescribed in advance. Universities teach though the knowledge currently available but the world of professional work in the future will be different from what is known about today. Hence graduates need to emerge from universities not just with a grasp of the current wisdom but with the capability to use that knowledge to solve new problems in new fields, acquiring more knowledge as necessary in the process. Bowden[8] has described that as knowledge capability, which enables the professional to see a situation, discern what are the relevant aspects, deal with those aspects simultaneously in formulating the underlying problem, and then use knowledge already gained and/or acquire any new knowledge necessary to solve the problem.

This is a development from basic variation theory[7,9] which argues that the ability to discern the relevant aspects of a situation cannot be developed unless variation is experienced (we don't become aware of our breathing until we enter a smoke-filled room). Students need to experience variation in contexts of problem solving so they can reflect on those variations, see what is common and what is different and understand why the differences exist. Approaches to learning that involve matching a learned set of problem types with a learned set of solution types should be discouraged. Students who have learned such a matrix of solution-types will have difficulty with an unknown type of problem in a context never experienced before. Variation theory would argue for comparison of different problem-solution relationships as part of the learning process, development first of all of an understanding of why the different approaches work in each context and secondly development of the capability to devise a solution method (i.e. not just choose one of those on the rote-learned list) when confronted with any problem, even if never seen before. So the current theory would argue for students to experience the variation rather than just having a varied experience. Experiencing realistic problem situations is one aspect. Reflection by students on their various experiences is another essential element. Assessment that reflects this perspective is also needed. This project begins from that theoretical base. Students will also be encouraged to monitor their own capability development through an electronic portfolio system that will assist such reflection.

Project objectives

The main goals of the project are:

- To evaluate the implementation of the new mathematics courses and their integration with the chemical engineering courses
- To help students attain a deeper learning approach to chemical engineering fundamentals including realistic modelling of scientific and technical phenomena
- To help students attain a deeper learning approach to mathematics using realistic chemical engineering examples
- To increase student independence by introducing more interdisciplinary assignments and projects
- To increase the possibility of introducing new and varied forms of teaching (and learning situations) in different courses

- To encourage a deeper understanding of the subject by introducing more appropriate assessment of student learning
- To make more effective use the mathematical skills in chemical engineering subjects

The means to achieve these goals are, for example, a team of teachers and creation of larger interdisciplinary and integrated courses (Mathematics/Chemistry/Chemical Engineering).

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:

- ensure that the prime focus is on understanding of the fundamentals and not simply on the algorithmic application of skills
- focus on how the views of the students and the teachers change regarding what is important to learn
- co-ordinate what, when and how to learn certain aspects
- assess changes in the workload of the teachers and students as well as in how they work
- investigate whether these pedagogical changes in the learning situation suit all types of students (gender, background, and prior experiences) and the effects they have on individuals
- explore to what degree we can efficiently use the new and more applied student knowledge in mathematics - how should we train, inform and prepare the teachers (and students) for this?
- examine the changes necessary to the assessment procedures to foster a deeper learning approach by the students.

One big question will then be: How do we measure good results in terms of increased understanding/ learning and capabilities? This is very hard to answer at the moment but some ways to examine this effect are to use the teachers´ reflection and motivated changes in teaching and learning methods and the type of student/teacher and student/student interaction as indicators of an improved learning situation. As in many pedagogical projects the process in itself is very useful when the teachers actually work (find time to engage) with development of their own teaching and ask questions such as: What phenomena can and will be described and may be learned in a different manner from before? Why, when and how?

Actual activities - Academic years 2001 - 2003

In the spring of 2001, team formation in the courses and integration of teachers in different and interdisciplinary courses took place, together with the planning and preparation of the fundamental chemistry and fundamental chemical engineering courses. This is completed for the chemistry course which started 2002. A large number of integrated parts (chemistry/mathematics) are now included in the whole chemistry course.

Integration of the Chemistry and Chemical Engineering subjects and their basic concepts and engineering problems into the mathematics has been performed on a number of courses in the year 2001/2002.

Workshops for chemical engineering teachers and students have been held.

For the Chemical Engineering subject, work is in progress (planning and producing course material). Some preliminary teaching projects in chemical reaction engineering have been executed and a preliminary evaluation undertaken

BIOENGINEERING EDUCATION

As a brief example of how a program is performed we use bioengineering. Biotechnology was begun in 1996 with 35 students taken in annually (now 70). In 2000 the first students from this program graduated and applied for positions in industry, research centres and universities. The related curriculum (which is under development) is shown in figure 1.

Figure 1 about here

From the last year a number of directions such as medical and molecular biology, food science, forest and environmental science and the more traditional bioprocess engineering sciences are possible.

The goals for this program are to:

- 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 skills
- 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

Given these engineering goals and aims for this program in view it is obvious how essential mathematics, and the use of mathematics for problem solving, is for the whole program.

MATHEMATICS LEARNING APPROACH

Virtual reality and computer based simulations bring 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, for example, bioengineering, environmental and chemical engineering, chemistry, economics 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 that 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 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; the new tools of calculation such as CMM/CAD will be very relevant in this context. This technology can be used to build links 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 modelling. The quality and level of mathematical learning determine the status of the total education. Modelling in the engineering subjects and education has changed towards the use and development of computers. An integrated education is therefore necessary for a successful engineering curriculum. This integration is planned and discussed in many technical universities at present. How much and what should be changed differ, according to whether one asks mathematicians or computer scientists.

Engineering subjects often consider today's traditional mathematics to be of little use for solving relevant engineering problems. Problem formulation and solution in these subjects have therefore been limited to analytical solutions. The new mathematics course at Chalmers is a synthesis of mathematical analysis, linear algebra, numerical computation, and application of mathematics to problems in science and engineering. In the traditional engineering mathematics course, the discussion is mainly limited to the special cases that can be solved by analytical methods. By taking a constructive approach, based on numerical computation, we can address equations (algebraic equations, ordinary and partial differential equations) in their general form. This allows us to discuss realistic engineering applications (reaction kinetics, chemical equilibria) already in the first semester, and to reach more advanced applications (convection-reaction-diffusion, fluid flow) in the second year.

Mathematics, numerical analysis, and programming are taught in an integrated way. The programming environment is Matlab, which is a software package for numerical matrix computations. It can be used at various levels; from a simple calculator to a rather advanced programming language. It contains tools for graphics and toolboxes for various engineering disciplines. In the early courses our students write their own programs for solving algebraic and differential equations rather than using the programs provided in Matlab. Writing programs is an essential part of our pedagogical idea; it forces understanding of the mathematics and algorithms, it also gives the student confidence in his or her ability to solve problems using mathematics.

In 2002 the first year of all Masters programs at the school of chemical engineering had been revised according to the ideas in the integration project. This was a necessity for the creation of a complete and successful, new basis for the interaction with all engineering courses in the second and third year and in order fully to use this new type of knowledge that the students have learned.

STUDENT INTERACTIONS IN MATHEMATICS

Every week the 185 students and teachers meet in 4-hour lectures (traditional), 4-hour computer studio classes (48 students), and in exercise classes of 4 hours in tutor groups (8 students), engaging in learning activities that include problem-solving, projects, and case studies with written and oral presentation. These exercise classes are led by two teachers, with one more experienced and the other a PhD student. Due to this high quotient between teacher and students the use of older students as junior supervisors will probably develop in the future. These exercise classes also give the students more time to reflect and solve problems early in their mathematical training. More applied examples are brought into the curriculum at an early stage. Material for the first courses has been developed in a new textbook[10]. A lot of additional course material is available on the course website[11].

Integration of chemistry and mathematics

This project focuses on how learning in chemistry can be improved by mathematics and vice versa.

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 difficulties in applying the mathematical methodology used in one area of chemistry to the development of knowledge in another area of chemistry and also in seeing the relation between different subjects of chemistry.

Thus it makes sense to integrate inorganic, organic, analytical and physical chemistry and at the same time focus on how mathematics helps us understand chemistry.

Example from chemistry mathematics integration

Kinetics project

That chemical reactions go at different speeds is mentioned rather early on in the course, but not developed further until after nine weeks. Then chemical kinetics is introduced in chemistry lectures and differential equations in the mathematics course. Whereas in chemistry we restrict ourselves to integrating the rate equations to get the concentration as function of time (the result useful in practical cases) for simple systems, the general treatment in the mathematics lecture shows (by among others chemical examples) how more complicated systems can be solved.

The students then get to choose from a selection of chemical problems too complicated (or time consuming) to solve by any of the methods given in their chemistry textbooks. During the following two-three weeks they work (usually in groups) on these problems, either on a few designated studio tutorials in mathematics or in the non-specific problem solving sessions in chemistry. Finally a report is handed in and marked by both a mathematics and a chemistry teacher.

Later on (weeks 15-16) we again come back to kinetics in the chemistry course, but then in the context of reaction mechanisms and use a more matter-of-fact application of the simple principles; we do not solve differential equations again.

Atomic and molecular orbital examples

Atomic orbitals are first introduced in the mathematics course early in the first semester in the context of the 'particle in a box'. Students learn to compute derivatives of the sine function and show that it satisfies the Schrodinger equation. They then interpret the function as a probability density, they normalize to unit total probability, they apply boundary conditions for the confined particle, discover quantization of energy, and define the spectrum as the difference between energy levels. This is then followed up in the chemistry laboratory, where the students measure spectra.

Molecular orbitals are encountered in the beginning of the second semester. When the students are familiar with the matrix eigenvalue problem, a chemistry teacher visits the mathematics course and lectures about the Huckel method, where molecular orbits are built up as linear combinations of atomic orbitals. This methods leads to a symmetric eigenvalue problem. The lecture is followed by a computer studio exercise, where the students set up and solve Huckel problems by hand for small molecules, by direct Matlab computations for slightly larger molecules, and finally for large molecules by means of the ready-made program Huckel lab. They compute spectral data for carotene and lycopene, which they bring to the following chemistry lab, where they isolate carotene and lycopene from carrots and tomatoes. The computed spectra are compared with measured spectra. These lessons and labs were planned and carried out by mathematics and chemistry teachers together.

EVALUATION

The evaluation of the first part of the project involved an iterative process in which independent evaluators established a base line for later comparison before the implementation of the new course. For example the twelve teachers involved in developing the new course were asked

- Why were they changing the course?
- What were the most significant changes?
- What benefits would the students get from the new course?
- How would they know the changes had been successful?
- What were the perceived strengths and weaknesses of the new course?
- How will they assess learning (including the alignment of assessment with course objectives)?

Eleven out of the twelve teachers gave detailed answers which matched, for the most part, the description of the project's aims, objectives and method of implementation that has been given above. Not everyone responded to the questions about assessment. This was raised in follow up interviews where it was revealed that not all teachers were clear as to who would be responsible for assessment procedures. This was sorted out later in the planning process. All agreed that changed assessment practices were the key to success but warned that some students were comfortable with traditional exams and would probably react negatively to the changes.

Students in the old program who knew about the proposed changes were also asked for their opinion. Twenty percent responded (about 40 students altogether) and gave comments as well as filling out a questionnaire. The majority thought the integration of the various chemistry disciplines into a common course was a good idea and approved of the idea of spreading the lecturing. Most of the dissatisfaction with the traditional large lecture course they had themselves experienced related to poor lecturing. They saw an advantage in smaller groups and more diverse lectures. They were positive about changes to assessment, especially varying it, but concerned that the proposed end-of-course, open-book exam that was designed to help students synthesise their learning would be too exacting.

The first year of the new course has been completed (May 2003) and the teachers surveyed again using the same set of questions. The new intake students have also been sent an email questionnaire which is still being processed. The teachers response has been very positive. They carried out their own evaluation of the course where students could voluntarily fill in a form on the web and all but two students thought the new course was a good idea. Ten (25%) thought that the implementation of the idea could be improved.

The student complaints, like the previous year’s cohort, often related to poor individual teaching performances. In this case the criticism focused on a particular group of teachers that insisted on teaching 'their own subject' only (a minor part of the course). This did not only break from the basic idea, but also meant that they were not involved in the 'team teaching' and evaluation process. This was probably the main cause for the poor performance of this group of teachers. Interestingly enough, this negative attitude from the tenured staff did not reflect on the graduate students during their supervision of the practical work who got excellent reviews from the students.

The main aim of the curriculum reform, the greater integration of chemistry disciplines and mathematics and chemistry, was successful according to both the internal evaluation and independent interviews with teachers. Some of the comments that students volunteered on the website survey were ‘Great idea to combine maths and chemistry’, ‘It’s good to see that what one learns in maths can actually be used in chemistry’, ‘Excellent with applications’ and ‘Some of the maths-chemistry projects were really good. It was good to see why maths is important and that early in one’s education learn to apply one’s knowledge’. In the new course chemists were available to help students during maths lectures. Two of the projects required students to solve problems of equilibrium using Matlab. There were some drawbacks that were revealed. Too much time was taken to solve problems in the independent projects and next year an extra tutorial will be introduced.

The examination results were not so different from the previous large lecture course. There was also a similar distribution of results with the program with much higher average grades from secondary school doing much better than the other programs. The touchstone of success will be the quality of learning that occurs in the new course. The perception of the teachers who are committed to the new curriculum is that it is better. Getting evidence for that, particularly from an analysis of student responses in the open-book exam and the oral tests is not so easy. The final open-book exam was considered a burden by a lot of students who would prefer to break the twenty one week course into smaller parts. ‘I thought the idea of a large, integrated basic course in chemistry was really good, but would rather see three smaller tests rather than one large one. I believe one would learn more at the end of the course if this were the case’. Perhaps this sentiment is partly a hangover from the more common smaller courses that students find manageable The idea of a final exam is to get the students to look back and review the whole course but the criticism is worth reflecting on. The responses that the evaluators received from both teachers and students at the conclusion of the new course showed that the idea of integration had worked. The main conclusion from the course evaluation was that the team teaching had been a great success and benefited both teachers and students. New initiatives take time to gain acceptance, especially in traditional institutions like Chalmers, but the indications are that the new program will enhance the quality of learning in undergraduate chemistry.

Academic year 2003 – 2004

For the academic period in 2003 and 2004, the intentions are to implement the new mathematics into the chemical engineering courses and vice versa. For the third and fourth year the following engineering courses are interesting for the continuation of the project. 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 one examples of what has been and can be achieved in these courses as a consequence of this new mathematics knowledge we consider the third year course in Chemical reaction engineering.

CHEMICAL REACTION ENGINEERING

The teaching in chemical reaction engineering (a central course in all the programs in the school) 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 encourage the students to approach the subject in a deeper and more fundamental way. The new preparation makes the subject more focused on discussing the phenomena involved in a more qualitative and basic manner. It is also possible to add new areas within the subject such as multiphase flow in different reactor configuration.

Figure 2 about here

Through the use of computers (now the students are used to applying computer science and mathematics for applied subjects) the teaching situation gradually is changing from developing analytical solution by dribble with mathematics to discussion of the problem formulation, solution and interpretation of the results. The possibility of getting the students to interact in a teaching situation more like their forthcoming work situation[8] 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 exposed in these simulations.

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

It is, furthermore, our belief 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[7,8].

Requirements for a successful project and generality of the project outcome

Figure 3 about here

Although this is a project in the field of integration of mathematics/numerical analysis with chemistry and chemical engineering, the outcomes and interpretation of the outcomes are of general interest and will be beneficial for all engineering programs internationally as well nationally. The project will show and describe effects of integration of many different subjects on how the students improve in learning involving

- Deeper understanding of basic phenomena,
- Improved relevant problem solving skills
- An engineering approach to attacking problems and also the critical interpretation of the results.
- The development of the student's ability to work independently.
- The student's appreciation of the main and basic fundamental aims of their education

In the end this and the way we assess the student will also lead to improved examination performance which is of general interest for all universities. We also try to focus in the evaluation procedure on how the integration project effects heterogeneous student groups which is of general interest for all pedagogic projects.

STUDENT PARTICIPATION

Student representatives have actively participated in the project by leading groups and contributing to many of the ideas in the project. The student union group at the school of chemical engineering has formed a team for discussion in this project (Notes are on the web page). The enthusiasm and work from the students is essential and highly appreciated in this project. Students are also involved in the pedagogical evaluation of the project and in the formation of questionnaires and so on. This project was designed to improve the quality of student learning in undergraduate chemistry at Chalmers. Such changes are difficult to measure even when sophisticated qualitative research techniques are used. What we can conclude and what we argue for in this paper is that an integration of mathematics and chemistry, where real life problems are solved using both disciplines, is better than separate doses of mathematics and chemistry where the student struggles to find a useful relationship between two sets of theoretical knowledge. Students and teachers, from different maths and chemistry fields, have worked together to improve a fundamental part of their engineering education. The result has been shared knowledge, greater practical application and an undergraduate chemistry course where real understanding of the subject is prized and promoted.

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Eng. Linda Hellström

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Fig 1

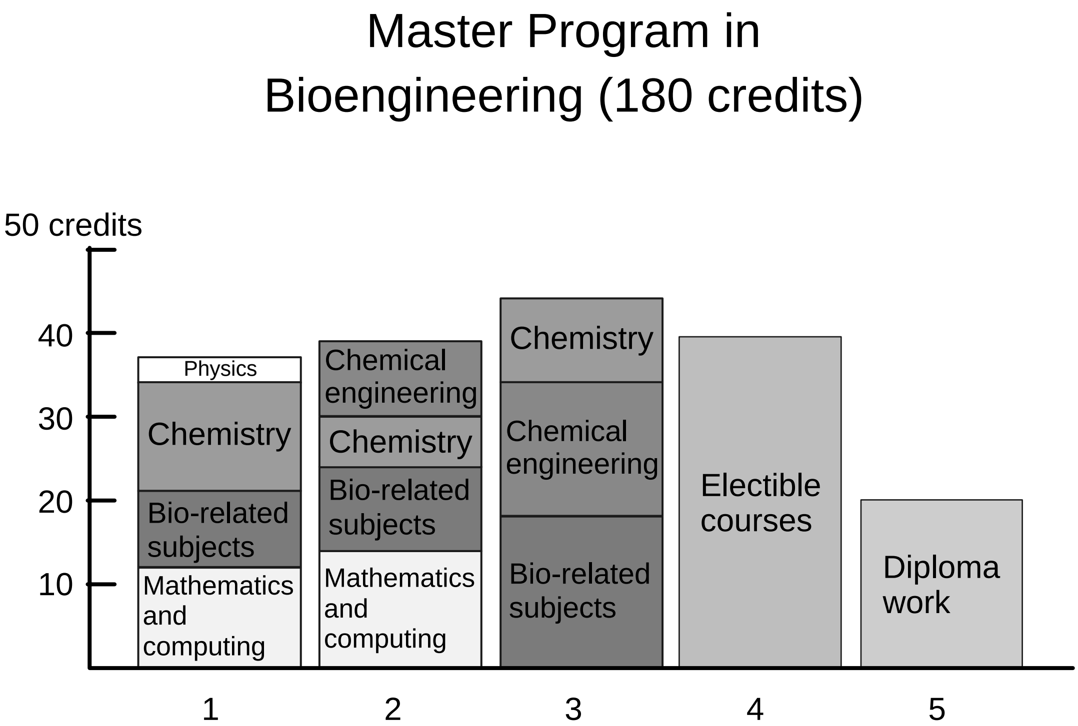


Fig 2

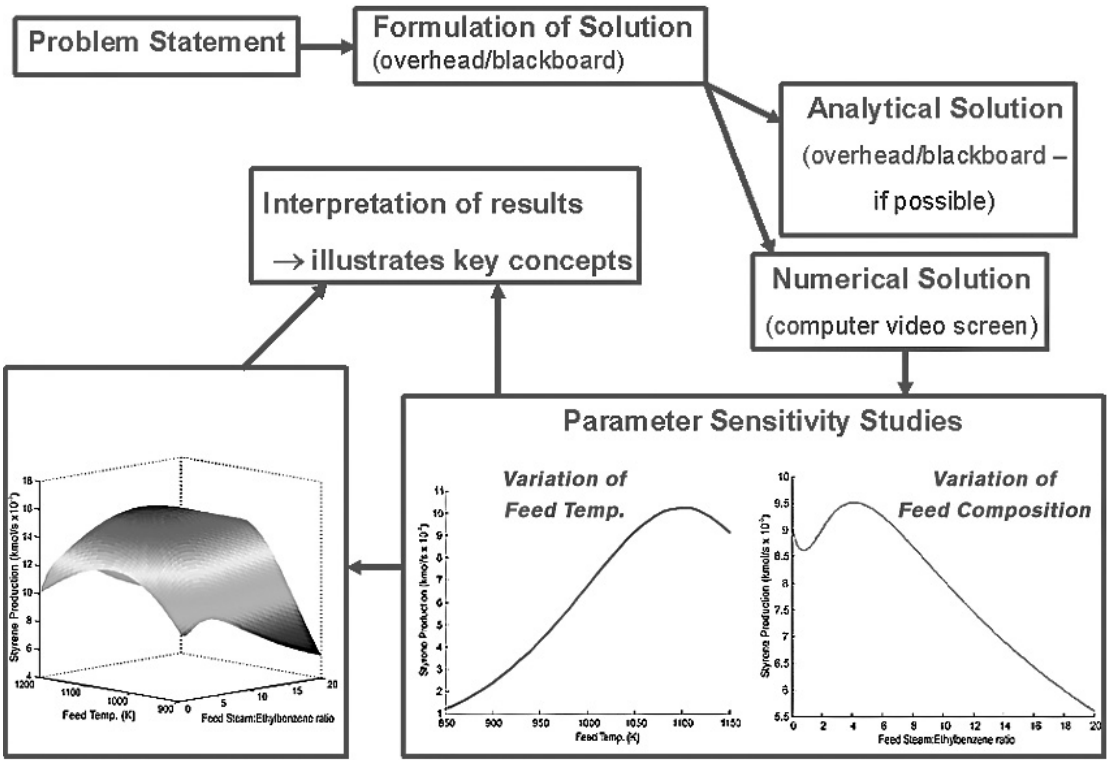
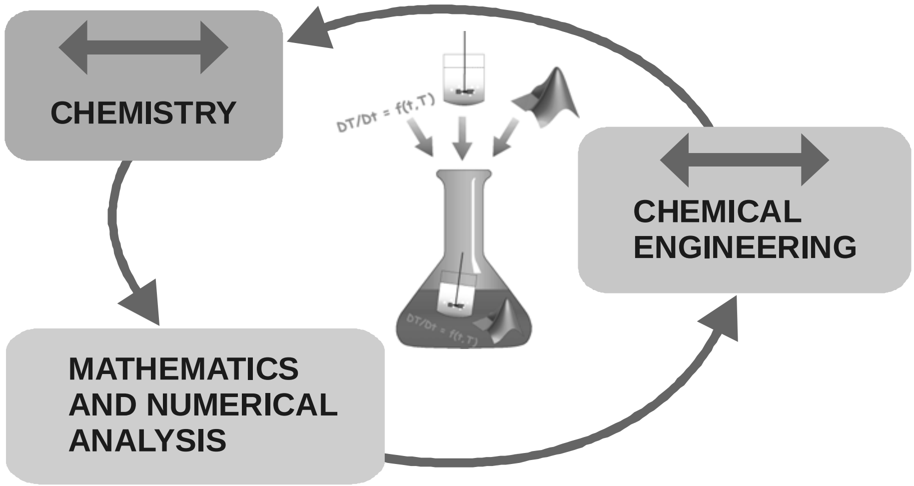

Problem Statement
Formulation of Solution
(overhead/blackboard)
Analytical Solution
(overhead/blackboard – if possible)
Numerical Solution
(computer video screen)
Interpretation of results
→ illustrates key concepts
Parameter Sensitivity Studies
Variation of Feed Temp.
Variation of Feed Composition
Feed Temp. (K)
Feed Steam:Ethylbenzene ratio

Fig 3


CHEMISTRY
DT/Dt = f(t,T)
CHEMICAL
ENGINEERING
MATHEMATICS
AND NUMERICAL
ANALYSIS