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PROFESSIONAL PAPER

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CHEMICAL ENGINEERING AND CHEMISTRY: EDUCATION IN A CHANGING WORLD

Current trends in science and engineering research are analyzed, together with an inventory of changes in the field of employment and practice in industry. The resulting demands on the university education of chemists and chemical engineers have been translated into a more or less continuous updating of the curriculum at the Department of Chemical Engineering and Chemistry of the Eindhoven University of Technology in the Netherlands.

In general it can be said that the emphasis within education will have to shift from the knowledge of facts, towards the ability to apply this knowledge to the process of solving problems in a realistic setting. Two topics will be highlighted.

Multidisciplinary project group work was successfully introduced to enable students to apply theoretical knowledge to real life situations in a professional (industrial) context, resulting among others, in a sharper focus on communication skills.

On the other hand, knowledge of theory and experimental practice are combined and augmented by the increased use of experiment simulations for illustration, demonstration, and experimentation purposes. Here, the increased use of information technology facilities and skills is essential.

The Eindhoven University of Technology (TU/e) was established as the second University of Technology in 1956. It is located on a compact campus with a considerable amount of green spaces in the center of Eindhoven, a town of 200.000 inhabitants in the southern part of the country. Eindhoven is the center of the most industrialized region of the country, technological industry accounts for 46% of the local productivity. There are 9.500 companies (such as Philips, DAF, ASML, Toolex, Simac, Neways and the research organization TNO), providing employment to more than 120.000 persons in the region.

The University has 9 scientific Departments and offers 10 academic three–year Bachelor programs, 19 Master programs (for the Dutch "ir" title), 10 two–year postgraduate design programs, 3 first degree teacher–training programs in mathematics, physics and chemistry, as well as various other postgraduate courses and four–year PhD programs. There are approximately 3000 employees, 220 professors, 6800 students, 200 postgraduate students, and 450 PhD students. Since its founding, TU/e has delivered 20.000 graduate engineers, 1000 postgraduate design engineers and has awarded about 2000 PhD titles.

One of the challenges in science and engineering education (and it can be extended to other branches of science) is best summarized as follows: our scientists and engineers of tomorrow are educated today, but those involved in teaching, were educated yesterday. One can also look at it from a different angle by observing that a university curriculum (excluding a PhD) in any branch of science has always been, presently is and probably forever will be approximately 5 years, whereas in the past decades the knowledge domain concerned increased progressively and the demands of society on our academics at the same time have not decreased, to put it mildly.

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TRENDS TO ACCOMMODATE

In order to cope with the challenges mentioned, those involved in science and engineering education should keep a keen lookout on trends in industry and on research in general. No science curriculum can afford to continue unchanged for a decade or more.

If we look at the knowledge domain in science, we can see it increase progressively. For example, the annual number of Chemical Abstracts increased [1] from 150000 in the 1960's to 600000 in the 1990's. Accumulated, this corresponds to a 10–fold increase during an average person's working life (Figure 1). Another trend is the one from generalist to super–specialist. Naturally, the universal medieval scientist avant–la–lettre, working on astronomy, alchemy and medicine at the same time has retired ages ago, but the trend for ever increasing specialization still proceeds and is best illustrated by quoting Price's law [2], indicating a doubling of the number of different scientific journals every 15 years, a trend that has been going on ever since the 18th century up to the present day (Figure 1). Only advanced electronic search facilities enable us to access at least some of the material accumulated. Obviously, the professional skills required have shifted from factual knowledge to skills of finding, selecting and applying that knowledge.

Increased demands for computer modeling, the technology push from information technology in general is increasing. Information overload is due to electronic journals, web technology, attention services of smart se-

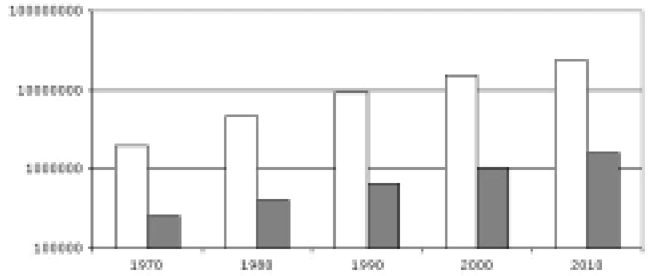

Figure 1. Logarithmic value of the accumulated number of Chemical Abstracts (white bars) and total number of different Scientific Journals (solid bars) within a person's working life.

arch engines and e–mail. Stating that all these new facilities have made all our lives easy is an over–simplification. The technical skills needed to fully use the opportunities of information technology should not be underestimated and all educational institutions, ranging from basic school to university should play their part. And according to Moore's law [3], information technology progresses even faster than science (doubling every 18 months).

When we look at the employment of chemical engineers and PhD's in industry, there is a trend away from traditional chemical companies to even larger conglomerates including the food, pharmaceutical, bio, fuel, and electronics industry [4]. The new employee entering the company is immediately immersed in a multidisciplinary environment, having to work together with team members with different scientific background (or lack thereof), level of education, seniority and culture. Both industry and academia are increasingly focused on internationalization, and the Bachelor/Master system of the Bologna treaty has stimulated student mobility in Europe, in addition to an increasing influx from non–EU countries.

There is yet another trend in the chemical industry at large: that towards the integrated development approach (IDA) to Process R&D [5]. The bottom line is that industry discovered the inevitable downside of super specialization. In industrial process development, there originally was a sequential chain of different groups where a discovery chemist worked out a discovery and threw it over the wall to the synthetic organic chemist, who handed the chemical over to the pilot plant engineer etc. The manufacturing engineer was the last one in the chain to make the product, in splendidly isolated ignorance of most of the experiences in the preceding chain. An integrated approach has now emerged where all of the people mentioned are more or less involved in several stages of development, cooperating in a multi disciplinary project group, of possible flexible composition in time. Obviously, this requires new skills from all those concerned.

RESULTING DEMANDS ON EDUCATION

It seems obvious that regular changes in science curricula are needed to cope with society's demands stipulated above. Feedback from the field of employment is therefore crucial. Several ways to do so include extended surveys of industrial research partners, and alumni. Especially the latter give valuable insight into possible deficiencies in the curriculum. Our Department chose to regularly (but not annually) adjust the curriculum according to the changing external demands, depending also on current didactical developments, and increased possibilities in information technology. In short: the approach is both customer driven and education driven, with a fair amount of information technology push.

Table 1. Education trends at the Eindhoven University of Technology

From	To
Knowledge of facts	Skills, competences (where to get & how to select info)
Isolated cases	Integrated approach
Guided exercise	Problem oriented approach
Passive attitude	Active educational setting
Individual work	Group work
Mono disciplinary	Multi disciplinary work
Mono cultural	Multi cultural environment
National context	International framework (Master in English)
Final examination	Life–long learning
Library instruction	Information Technology skills

Some of the resulting trends in the educational setting at the Eindhoven University of Technology are indicated in Table 1. These trends are not typical for our University: they are observed in many other educational institutions the world over, albeit to different extents and at different paces. The current paper will highlight two different aspects in more detail: group work and the use of information technology. The focus will be multi disciplinary projects and the use of computer simulations of experiments.

GROUP WORK

Within the many different forms of individual educational settings (attending lectures, doing exams, term papers, assignment) group work up to the 1970's has played a negligible role. At the Department of Chemical Engineering and Chemistry, only experimental work in undergraduate courses was performed in pairs of 2 students, for the sole non–didactical reason of efficiency (time and money). In the late 1970's group work was successfully introduced in the 1st year, within the framework of a Science and Society project. In the 1990's, a multidisciplinary project was introduced in the 4th year (of a 5 year curriculum), presently in the Master program. Last year, the whole Bachelor program was revised, with design–based learning projects in each semester. At present, group work amounts to about 25%

of all educational activity. The industrial internship and the graduation work (and possibly PhD), however, remain individual activities and exams are still considered essential. Other departments in Eindhoven, have taken a more extreme route: the newly established Industrial Design has no individual exams at all and both Mechanical Engineering and Biomedical Engineering have significantly more group work than our department.

Multi disciplinary project groups were introduced in the 1990's. At present they are coordinated by an inter–department center [6], and several Departments participate and exchange students. The project has 8 credit points and is situated in the Master program of the participating departments. The educational goals [7] can be summarized as follows:

- Cooperate in a team with students with different specialization. Deal with practical problems (problem definition and analysis). Combine existing technical knowledge. Locate and acquire and apply new information. Independently incorporate non–technical aspects (any...)
- Project work (planning, phasing, monitoring progress, costs...)

Depending on the subject, additional technical goals can be set. The project result is always a report and a presentation, sometimes also a web–page [8], sometimes a working prototype or experimental results, a poster presentation on a student conference [9] or even an article in a scientific journal. Intermediate results may consist of a project plan, interim reports, interim presentations and such like.

The organization has the following time frame: 8 weeks prior to the start of the new semester, project subjects are listed on a university website [7], including the following information:

- Title and Description
- Organizing Department
- Staff member or external client responsible
- Specific requirements relating to the subject
- The desired group size and departments for which it is intended

During a 4–week period, students can register with a web form, stating three preferences for projects. Two weeks before the semester starts, group compositions are made, based on student preferences, priority of projects and other boundary conditions relating to group size and composition. The final decision is made at a meeting of coordinators from the departments involved. Typically, 70% of the students can be accommodated in a project of their first preference, the remainder on their 2nd or 3rd preference.

Each department has its own organization of these projects. These organizations inevitably differ in detail, depending on the size of the department, the place of the project in the curriculum, the parties or persons involved, the kind of subjects preferred and the facilities available. As an example, the situation at the Chemical Engineering Departments is further illustrated [10,11]. We started in the early 1990's with a multi disciplinary pilot–project as an optional course for chemical engineers. It was soon afterwards made compulsory, and mixed teams from different departments are now regular practice.

The following roles in the project organization can be distinguished:

- The Client is the person(s) proposing the subject, who is by commitment interested in the outcome of the project. This is often a staff member or someone from a company.
- The Group of students, who among themselves elect a project leader and a treasurer. A Chairperson and Secretary in group meetings is rotated between group members
- A Tutor, who monitors the quality of the group process and individual performances therein, intervenes if necessary and together with the Client plays an important role in the grading. The tutor typically is a PhD student, who for this task has been given previous training.

Project subjects are proposed by university staff members or external partners, e.g. from industry. In several cases, part–time professors proposed subjects originating from their company. Generally, one may divide the subjects into one of the following four categories, as illustrated by a typical example:

- Feasibility study: e.g. A new type of glass has been chemically modified in such a way that interesting additional properties are obtained. What potential areas of application for this material in biomedicine would be most promising? (Client: Department professor)
- Scenario studies: e.g. In a long–term EU strategy, in the year 2020 at least 10% of the electricity should be generated in a sustainable manner. Investigate how this could be technically implemented using bio–fuel. (Client: Center for Sustainable Development6)
- Prototype design studies: e.g. Design, build and test a refrigerator that works on solar energy, for application in remote areas of developing countries [10]. (Client: Company manufacturing Stirling engines)
- Business plan: e.g. There is an increased miniaturization of intelligent "smelling" devices. What are the commercially most promising high–volume low–cost consumer applications in combination with existing communication technology? (Client: Electronics company).

Experience from past years has indicated that both the group process and the result gain huge benefits from the interdisciplinary approach. In addition, the organization has proved to be able to incorporate distance co–operation with departments at other universities, and to include the international Master students as team members, resulting in a highly motivating challenge to all concerned, and providing an excellent preparation for a professional engineering career in an international and inter cultural context. We are convinced that the present scheme (depending of course on the subject of the project) can also be extended to or implemented in non–science disciplines. More details on this can be found in a dedicated paper [11].

With regards to international aspects of cooperation in multi disciplinary project work, another dedicated paper [10] has dealt with the extended use of information technology for communication purposes [12]. This fits in nicely with the growing importance our University attaches to using these techniques in the educational setting on the campus as a whole.

USE OF INFORMATION TECHNOLOGY

As a result of the advance of information and communication technology (ICT) on society in general, during the 1980's and beyond, personal computers have also penetrated into all corners of University life. Providing access to PC's through the University networks for all staff members and students subsequently became an increasingly frustrating financial and logistic burden. In 1997, the University board decided for a revolutionary approach: the so–called "notebook project". Teaching rooms with outdated PC's were cleaned out, huge investments were made in network connections (nowadays largely wireless LAN), and all students were provided with a state–of–the–art (portable) notebook computer. The university and the student financed the latter jointly. A separate organization was set–up for purchasing the notebooks with a significant discount, for servicing and arranging for a favorable bank loan for the students, payable in installments. The project is still quite successful and has been copied by several other Universities in the Netherlands.

In addition to that, the University departments invested in the extended use of ICT in the educational setting. Student exam results are sent by e–mail, each student can access his own progress by logging in into the database. Most reports, essays and term papers are submitted electronically. All courses have full info on the web [12] (basic info such as content, lecture schedule), at Chemical Engineering and Chemistry, course WebPages [13] may include all material used Powerpoints, course guides, Word documents, PDF's, computer animations and simulations, interactive web–based self–tests etc). In addition to that, there are public folders in Outlook, also for teacher–student interaction and cooperation between students. The latter enable groups of students to work in virtual project rooms [14]. Other digital learning environments, such as Blackboard, offer these and other facilities.

The use of computers in experimental work, traditionally an important part of the curriculum, has increased enormously: most experiments can hardly be carried out without some form of embedded software or external computer control and data handling. Data handling in the 1980's, when intelligent data handling software was still in its infancy [15], the user had to be trained in that as well. For that we have been running a special practical course in signal processing, using simulation software [16–18]. As intelligent data handling software in the late 1990's became readily available, this course became superfluous. As mentioned above, most practical courses have experiments carried out by pairs of students, not for didactical reasons, but because experiments are expensive, both in time and money. In addition to that, experiments can fail, and are restricted in terms of safety, chemicals and laboratory locations and hours.

During the past decades a considerable number of real experiments have been complemented, extended and sometimes even partly or totally replaced by experiment simulations. Some examples in both Chemical Engineering and Chemistry will be illustrated.

Starting in the early 1960's, an essential part of the chemical engineering curriculum consisted of working in 3 eight–hour shifts for a week, in a small plant. The plant comprised a cyclic process of dissolving Na_2SO_4 in water, and through a series of unit operations evaporating the water to finally obtain the dry salt from a rotary kiln. The plant was not automated at all, so that a steady state had to be obtained and maintained manually, preferably optimized for yield. An essential part of the exercise was making several mass balances, sometimes by measuring an indirect variable such as temperature, not a straightforward job under fluctuating operating conditions. Our students were in fact trained to be an operator in a (old fashioned) chemical plant. When equipment wear and increased safety awareness in 1987 necessitated complete rebuild, it was decided to replace the plant with a simulation in ChemCad [19] (PC version). By that time operators in industry were already working in the control room of automated plants. In our department, emphasis increasingly shifted towards process design. Meanwhile AspenTech [20] was founded in 1981, with the objective of commercializing technology developed as part of the Advanced System for Process Engineering (ASPEN) Project at the Massachusetts Institute of Technology. Only in the late 1990's was the ASPEN software made available as a PC version, and since ca 2000 ASPEN is part of the basic chemical engineering software package running on student notebook computers. The program is fully integrated in both bachelor and master process engineering courses, using a dedicated textbook [21].

In a freshmen's practical course since the 1990's, introducing the basic concepts of chemical reaction engineering, an experiment with a three–phase stirred tank batch reactor is carried out. Glucose in water is oxidized at constant pH and temperature, using a Pd/C catalyst and oxygen from air in a 1 liter CSTR. Conversion is monitored using automated titration with NaOH. Conversion to 50% typically takes an hour and the equipment costs typically 10000 euro. The experimental setup is schematically depicted in Figure 2.a.

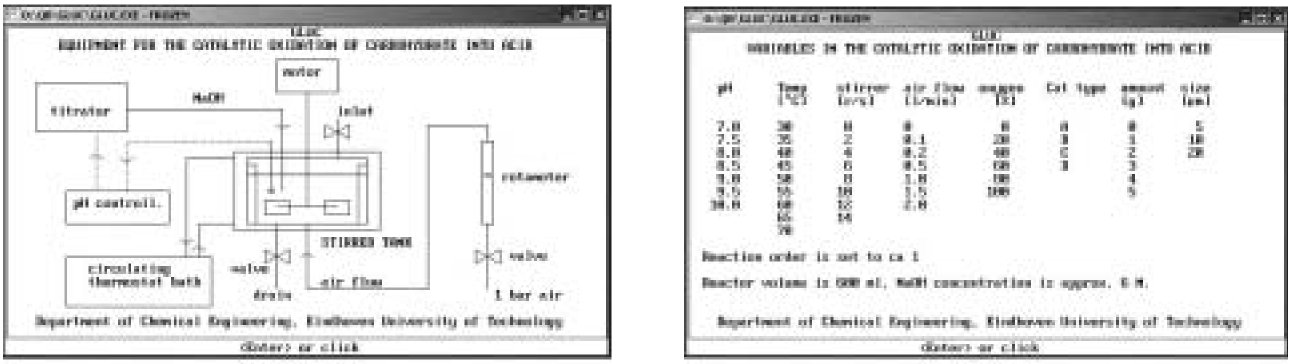

Figure 2. Glucose oxidation in a batch reactor, left (a) the experimental setup, right (b) the variables to be changed in the simulation and their range.

What is to be calculated is the reaction rate and order, and the activation energy. Measuring at three temperatures obviously fills the whole afternoon, the larger part of which is spent in waiting for the next measuring point to be read from the automated titrator, from which the conversion is calculated. Because a number of other interesting parameters were available, pH, initial concentration, stirring speed, air flow and the amount and type of catalyst (e.g. particle size, shape, solid vs. totally porous), it was decided to make an equipment simulator [22]. While waiting for the conversion in the real experiment to proceed slowly, several virtual experiments could be carried out with the simulator, so that a considerable number of assignments could be completed in the same time frame. The parameters to be chosen (see Figure 2.b) enable 1.5 million different experimental conditions. Naturally, only a fraction, but still a considerable number of useful combinations could be combined into interesting assignments dealing with one or more isolated aspects, such as mass transport limitations or characterization of the catalyst. The type of catalyst, for example, ranged from solid spheres to totally porous spheres, and the amount of catalyst could be changed independently of the particle size (Figure 2.b). The output screen of the simulator looks like Figure 3. The conversion X is plotted as – ln (1–X) vs. the reaction time, the parameters are shown top left. Naturally, the simulation is a speeded–up version of the actual reactor, in this case by a factor 6.

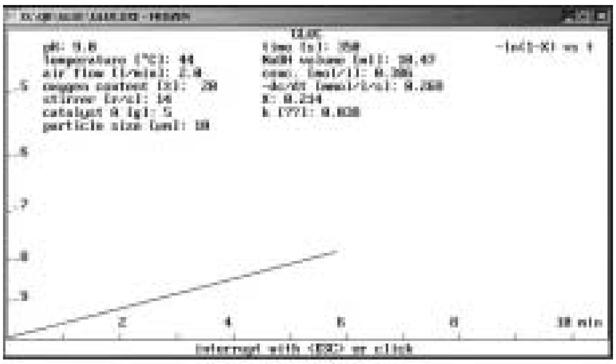

Figure 3. Glucose batch reaction simulator output example

Summarizing we can say that in general real experimentation, in combination with computer simulation makes it possible to efficiently use the time allotted for practicals, and to do more meaningful experimental work with less (expensive) equipment. In addition, practical assignments can in fact be carried out anytime, anywhere, individually, using the IT infrastructure available.

The power of simulations in an educational context is by no means limited to chemical engineering. In the area of chemistry increased use is made of advanced (and thus expensive) instrumentation, both for the qualitative characterization and for the quantitative determination of sample mixtures. Introductions to theoretical aspects of e.g. analytical separation methods are provided (either in lectures, instructions or guided self–study) and introductory experiments for each technique are subsequently carried out. In order to facilitate analytical chemistry training, a number of instrument simulators have been developed over the years, not as a replacement, but supplementary as a demonstration, and instruction tool, and as a first step in optimizing the separation of a given sample mixture. The resulting virtual laboratory now consists of GC, Capillary Electrophoresis (CE) [23,24], MEKC and HPLC.

Basically, the simulator generates a detector output signal, e.g. a chromatogram or, in the case of CE, an electropherogram (Figure 4). Parameters that can be changed relate to the sample mixture and to all equipment settings (injection volume, column specifications and dimensions, detection etc.). After each change a new output signal is immediately calculated and displayed. The number of parameters that can be changed is much larger than in the case of the simple chemical reactor simulator discussed above. As a result, the possible number of combinations of sample and equipment settings runs into billions.

Next to the above mentioned simulation software, developed in–house during the past decade, there are several other commercially available simulation tools for analytical chemistry, but these are not stand–alone simu-

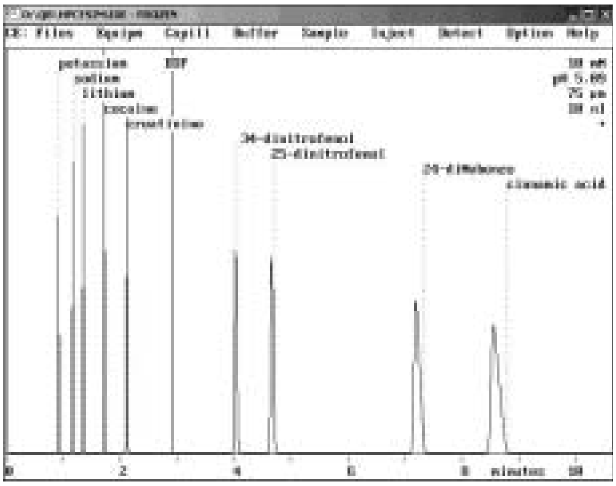

Figure 4. Result of CE separation of a model mixture with the positive cations move before the electro osmotic flow marker (EOF) and the anions, due to their negative charge move behind.

lators. The exception is ProteinLab [25], which is really quite complementary to the programs mentioned above: it integrates a number of analytical and preparative techniques specifically intended for proteins. Companies such as Academy Savant [26] have teachware: interactive textbooks with animations and a few simulations. ACDlabs [27] has GC and LC prediction software, where the prediction is based on previous experimental results, to be imported into the program. A product such as Chromsword [28] is likewise coupled to HPLC equipment, because it also requires experimental input to be extrapolated towards non–verified experimental conditions. In addition to that, the latter program is neither intended nor suitable for didactical purposes. Dedicated instrument simulators on the other hand, in addition to experimental work, can provide a valuable training tool in the analytical laboratory. Naturally they are perfectly suitable for demonstration and illustration purposes in almost any educational setting.

The instrument simulators discussed above behave in fact like an advanced instrument, because it instantly shows detector output. Other types of simulators intend to visualize what happens locally, on a smaller time– or distance scale. These simulators are perfectly suitable to show the dynamics of e.g. the separation in capillary electrophoresis [29–31].

CONCLUSIONS

Trends in industry, science and society but also feedback from alumni surveys have required regular adjustments to our chemistry and chemical engineering curriculum. Some of the major changes have been highlighted. Both relate to radical changes in the way of working in a professional context, as compared to the 1970's and 1980's.

These changes have forced us to focus on an integrated approach and increased emphasis on group work in multi disciplinary contexts. The fact is that this requires increased cooperation between departments but also with industry and other universities the world over. Our department considers these requirements a challenging opportunity.

Advances in information technology in general, and dedicated simulation software in particular have provided us with valuable tools in the educational process, in order to provide our students with relevant competences of increasingly complicated experimental and theoretical concepts, as well as data retrieval from the exponentially increasing domain of scientific knowledge.

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IZVOD

HEMIJSKO INŽENJERSTVO I HEMIJA: OBRAZOVANJE U SVETU KOJI SE MENJA

(Stručni rad)

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Postojeći trendovi u nauci i inženjerskom istraživanju su analizirani uporedo sa skupom promena u zapošljavanju i praksi u industriji. Rezultujući zahtevi za Univerzitetsko obrazovanje hemičara i hemijskih inženjera su pretočeni u manje–više kontinuirane promene nastavnog plana i programa na Fakultetu za hemijsko inženjerstvo i hemiju Tehničkog Univerziteta u Eindhovenu (Holandija).
Uopšteno se može reći da će se akcenat u obrazovanju morati pomeriti sa znanja i baratanja činjenicama ka sposobnostima za upotrebu i primenu znanja pri rešavanju problema u okruženju koje podražava realne uslove. Dve teme će biti posebno naglašene.
Rad u grupama koje se bave multidisciplinarnim projektima je uspešno implementiran sa ciljem premošćavanja razlika između teoretskog i primenjenog znanja za rešavanje problema u stvarnim situacijama. To je, između ostalog, rezultiralo u obraćanju više pažnje na komunikacione sposobnosti.
Sa druge strane, razlike između teorije i praktičnog rada su prevaziđene intenzivnijom upotrebom simulacija za ilustrovanje i demonstraciju eksperimenata, kao i za sam eksperiment. U tom slučaju organizovanija i učestalija upotreba informacionih tehnologija i sposobnosti je posebno važna.

Key words: Chemistry • Chemical engineering • Education • Trends • Group work • Projects • Experiment simulation •

Ključne reči: Hemija • Hemijsko inženjerstvo • Obrazovanje • Promene • Grupni rad • Projekti • Simulacija eksperimenta •