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Integrated Product and Process Development Using Case Studies: A Challenge to the Education of Science and Engineering Undergraduates

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Abstract. The education in integrated product and process development is a challenge for teachers, teaching assistants, as well as for students. At the Swiss Federal Institute of Technology, a new course in 'Safety and Environmental Protection Chemistry' has been established. To practise and exercise the tools introduced in the lecture, four different case studies of chemical products and processes have been developed in collaboration with the chemical industry. The subjects of the case studies are the insecticide Pymetrozine, the reactive dye Cibachron-LS, the red pigment DPP, and Perchloroethylene for dry cleaning. Various teams formed out of students from chemical engineering, chemistry, and environmental science work on topics like process safety, product safety, product risk assessment, and social responsibilities of manufactures. Different resource materials and guidance by a teaching assistant were provided. Finally, the students presented their results to industrial experts and received at the same time valuable feedback about the industrial approach to such problems. The application of the tools for integrated product and process development to actual case studies widened the students' scope of safety and environmental protection in a new proactive direction by a risk-oriented design of chemical technology.

1. Introduction

The chemical industry faces the challenge of optimizing chemical processes and products over their entire life cycle with the aim of minimizing risk, resource depletion, emissions, and waste. Chemical engineers and chemists are forced to recognize potential impacts as early as possible in the development of new processes and products. Because of changing regulations and a growing awareness for social responsibility, sustainability, and efficiency, the demand for integrated product and process development is increasing. Consequently, future chemical engineers and chemists need to be equipped with broader backgrounds in subject areas such as toxicology, environmental chemistry, economics, and the social sciences. Only so can the interdisciplinary evaluation of products and processes requiring, *e.g.*, redesign, reduction of energy consumption, reduction of toxic chemicals, cleaner practice in production facilities, and the environmentally conscious handling of products be tackled in a professional and effective manner.

Because integrated product and process development confronts scientists and engineers with a new conceptual framework that combines traditional with unfamiliar subject areas, training and education require an interdisciplinary approach. At the Swiss Federal Institute of Technology in Zürich, a new course entitled 'Safety and Environmental Protection in Chemistry' has been developed. This mandatory course is part of the core *curriculum* of 7th-semester undergraduates in chemical engineering, chemistry, and environmental science (chemistry option) and is the third in a series of three courses in environmental chemistry (*Table 1*). The new course aims to build on the scientific skills and backgrounds acquired in the courses Environmental Chemistry I and II, and enables students to professionally apply their knowledge to realistic problems [1].

The course in 'Safety and Environmental Protection in Chemistry' is divided into three parts: *1*. General Concepts and Backgrounds, *2*. Methodology and Tools, and *3*. Case Studies. Whereas parts *1* and *2* are held as two-hour lectures over a period of 14 weeks, part *3* is designed as a parallel, interactive program that focuses on an industrial and realistic project.

Table 1. *Three Courses in Environmental Chemistry*

Environmental Chemistry I: Chemical Ecology	
	Behavior and distribution, fate and exposure of organic and inorganic chemicals in the environment
Environmental Chemistry II: Toxicology	
	General concepts of toxicology, testing methods, and discussion of specific toxic chemicals
Environmental Chemistry III: Safety and Environmental Protection in Chemistry	
	Integrated process and product development, and the application of knowledge and basic concepts in cas studies

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Part *3* needs another approximately two hours work per week over a period of 9 weeks [2].

To assure the interdisciplinary framework for the case-study program, many different experts from chemical industry and academia had to be involved. These experts were essential for the design and review of the case studies. The participating experts work in such fields as the history and philosophy of science, environmental chemistry, toxicology, humanities, teaching and learning, and integrated process and product development.

2. Goals of the Case Studies

The acquisition of knowledge may be achieved in different modes. In the traditional mode, the students are taught the knowledge base of single, individual scientific disciplines like biology or chemistry or mathematics. This mode fails once complex problems have to be solved: *e.g.*, global warming, abiotic resource depletion, environmental pollution, and – an example of direct relevance to the new course – risk assessment of chemical products and processes. In such cases, a *transdisciplinary* approach is called for [3]. It is by working on the case studies prepared for part *3* of the course 'Safety and Environmental Protection in Chemistry' that the students are exposed to this new mode of knowledge production. They thereby have an opportunity to learn the following:

a) The practical application of concepts and assessment methods presented in the lectures;
b) the evaluation of product and process safety using appropriate methods and tools;
c) the analysis of complex problems and relations whilst working in interdisciplinary teams, and at the same time learning to manage their time effectively and to choose relevant strategies;
d) the recognition of their responsibility towards economic, ecological, and societal needs, and to be able to assess possibilities to influence them;
e) the presentation of their results and conclusions in a clear and integrated manner.

Table 2. *Overview of the Four Case Studies*

Case study 1:	*Pymetrozine* Pymetrozine is a new insecticide with a new mode of action. It is highly effective against aphids and whiteflies [4].
Case study 2:	*Reactive Dye* Cibachron-LS, a dye for cotton, has a bi-reactive binding mode characteristic and shows improved performance in the dying process [5].
Case study 3:	*Red Pigment* DPP ('Diketo-Pyrrolo-Pyrrole') is a new red pigment in paint for cars, *etc.* [6].
Cas study 4:	*Dry Cleaning* Tetrachloroethene (perchloroethylene, PER) is widely used as solvent in dry cleaning [7].

Table 3. *Tasks in the Case Study Pymetrozine*

Production process

1. Qualitatively evaluate the safety of the production process under the following aspects: process safety, environment protection, and occupational health. Identify key problems using the reaction and mass-flow diagrams provided. Suggest appropriate measures to reduce risk for normal operation and accidents.

Pymetrozine – the product

2. a. Discuss the following key properties and their importance for the sustainability of Pymetrozine: application quantity, acute and chronic toxicity, selectivity, persistence, water solubility, leaching into surface water, bioaccumulation, *etc.*
   b. Compare the key properties of Pymetrozine with those of Sukmeron.
   c. How could changes in the molecule of Pymetrozine affect its key properties?
3. a. Carry out a risk assessment for Pymetrozine using the results from task 2.
   b. Compare the risk assessment of Pymetrozine with that of Sukmeron.
4. a. Review the following aspects in the light of the responsibility of the manufacture towards ecology, economy, and society:
   – high-value product *vs.* the financial situation in third-world countries
   – minimized 'time-to-market' *vs.* long-term impacts
   b. Analyze which innovation goals have been reached in the development of Pymetrozine. Which additional goals should be pursued for a new insecticide?
   c. Using the data provided, list the arguments for and against the production of Pymetrozine from economic, ecological, and societal points of view. Assess their potential influence on the research and development process.

3. The Case Studies

So far, four different case studies have been developed (*Table 2*). All are based on actual products and processes from today's chemical industry. Information and materials were made available by the different chemical companies. The fact that all projects are based on real and actual problems was essential for the success of the program.

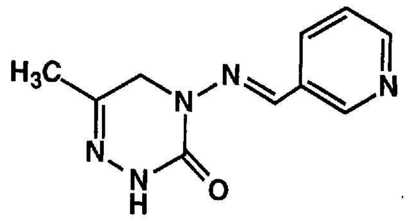
Every winter semester when the course is held, the students may choose one of the case studies (*Table 2*). Each case study focuses on a different category of chemicals that presents various key problems in safety evaluations. In the following part, the subject, the framework, and some examples of evaluated aspects of the case study 'Insecticide Pymetrozine' are described in more detail. For the other case studies, a brief outline of the essential features is given.

Case Study 1: Insecticide Pymetrozine

For the nutrition of a continuously growing world population, agrochemicals for plant protection are of primary importance (world sales revenue in 1993: 31 billion CHF). Each product has properties which are beneficial on one hand, but give rise to side effects for man and the environment on the other. Problems in plant protection include selectivity, persistence, residues in food and environmental compartments, resistance, and coproducts. Nowadays, it is the goal of the chemical industry to minimize these negative side effects.

Pymetrozine is an insecticide which is highly active against susceptible and resistant aphids and whiteflies in vegetables, ornamentals, cotton, field crops, and fruits. The compound affects the behavior of homopterous insects and causes them to stop feeding before they die.

One purpose of the case study is to check whether the development of Pymetrozine met the aspired innovation goals such as the social acceptance of insecticide, the protection of beneficial arthropods, the compatibility with Integrated Plant Production, low application



Pymetrozine

quantities per area, low costs, low mammal toxicity, low bird and fish toxicity, no cross-resistance, and low environmental impacts (bioaccumulation, degradation, *etc.*). In the case study, Pymetrozine is compared with another insecticide 'Sukmeron' (fictitious name), which was introduced in 1964. Sukmeron is also active against aphids. It is a carbamate and inhibits the essential enzyme acetylcholine esterase. Students had to conduct a risk assessment for the entire product life cycle using Sukmeron as a reference (*Table 3*) [8].

In the following section, examples of students' results and conclusions are summarized [8]. The final reports were much more detailed and comprehensive.

Process Safety

In the synthesis of Pymetrozine, phosgene is used for the ring closure of acetylhydrazine. Phosgene is very reactive, with water producing CO_2 and HCl. Because of its gaseous nature and the formation of HCl upon contact with water, phosgene is highly toxic, causing pulmonary oedema (TLV 0.1 ppm). The proposed safety measures include *in situ* production of phosgene, working within containments, installation of gas detectors, establishment of a safety zone, protection of eyes and skin, and the use of an independent breathing system. The suggestion of *in situ* production leads to an integrated approach, reducing the potential risk at the source.

Product Safety: Key Parameters – Toxicity and Ecotoxicity

The selectivity of Pymetrozine focuses only on homopterous insects. Since the control of pests is possible with low concentrations, the protection of beneficials is ensured (*Table 4*). Furthermore, due to no cross-resistance, the activity is efficient and durable.

Pymetrozine has a significant lower acute and chronic toxicity than the reference compound Sukmeron. The low persistence indicates that Pymetrozine is degraded readily in soil. The bioaccumulation is lower than the critical value of log $P_{ow} = 3$ (EEC-guidelines) and hence does not predict any accumulation effects in animals or humans. In general, the physicochemical properties, the toxicological and the ecotoxicological data show remarkable improvements.

Risk Assessment: Acute Toxicity

First, the acute toxicity of Pymetrozine is significant lower than of the conventional insecticide Sukmeron. Second, according to the guidelines of the European Union (EEC-guidelines), Pymetrozine is classified as 'non-hazardous to human health' because LC_{50} (24 h, rat, oral) is greater than 2000 mg/kg. And third, Pymetrozine causes neither eye nor skin irritation, nor mutagenicity, nor teratogenicity, nor carcinogenicity. Hence, Pymetrozine is a safe product for handling by humans.

Risk Assessment: Consumer Safety

In the case-study handout, the average food intake and the determined residues of Pymetrozine in food are given. Calculations with these data gave a Theoretical Maximum Daily Intake (TMDI) of 0.098 mg per person and day. The lowest, long-term toxicity value given in the handout was the toxicity for dogs (oral, NOEL, 3 months) of 3 mg/kg. Because no chronic toxicity values over a testing period of two years were available, the safety factor of 1000 might be appropriate. The resulting Acceptable Daily Intake (ADI) is 0.003 mg/kg·day and the Maximum Permitted Intake (MPI) per person is 0.18 mg per person and day (body weight 60 kg). The TMDI makes up only about 55% of the MPI. Therefore, the consumption of food treated with Pymetrozine has a low risk for humans. However, the discussion of scientific uncertainty is especially important for long-term effects.

Responsibility towards Third-World Countries

Pymetrozine presents the possibility to selectively control insects which are destructive pests in third-world countries, where crops like rice and citrus fruits are very important for the economy. Whereas in the past, widely active insecticides such as phosphoric-acid esters had to be applied, new products like Pymetrozine have the added advantage of lower environmental impacts alongside specific activity. However, the major hurdles are whether these products are available and whether they are affordable by the farmers. Because the application cost of Pymetrozine is relatively high (*Table 4*), the product can only be used by a small number of

Table 4. *Comparison of Pymetrozine with Sukmeron*

	Pymetrozine		Sukmeron	
Activity (14 days after treatment, same application quantities)	Aphids (*Myzus persicae*) 95%		Aphids (*Myzus persicae*) 45%	
Selectivity				
Pests	*Myzus persicae* LC_{50}	0.2 mg/l	*Myzus persicae* LC_{50}	7 mg/l
Beneficial arthropods	*Orius majusculus* LC_{50}	> 8.1 g/l	*Orius majusculus* LC_{50}	> 0.16 g/l
Acute toxicity	LC_{50} (rat)	5820 mg/kg	LC_{50} (rat)	100–200 gm/kg
Aquatic toxicity	EC_{50} (daphnia)	> 100 mg/l	EC_{50} (daphnia)	0.2 mg/l
Persistence (soil)	$t_{1/2}$	3–9 d	$t_{1/2}$	7–234 d
Bioaccumulation	log P_{ow}	0.2	log P_{ow}	1.8
Cost of application				
Switzerland	Potatoes	130.– CHF/ha	Potatoes	80.– CHF/ha
Egypt	Potatoes	65.– CHF/ha	Potatoes	10.– CHF/ha

LC_{50} = lethal concentration for 50% of the species; EC_{50} = effect concentration for 50% of the species; $t_{1/2}$ = half life (in days); P_{OW} = octanol-water partition constant.

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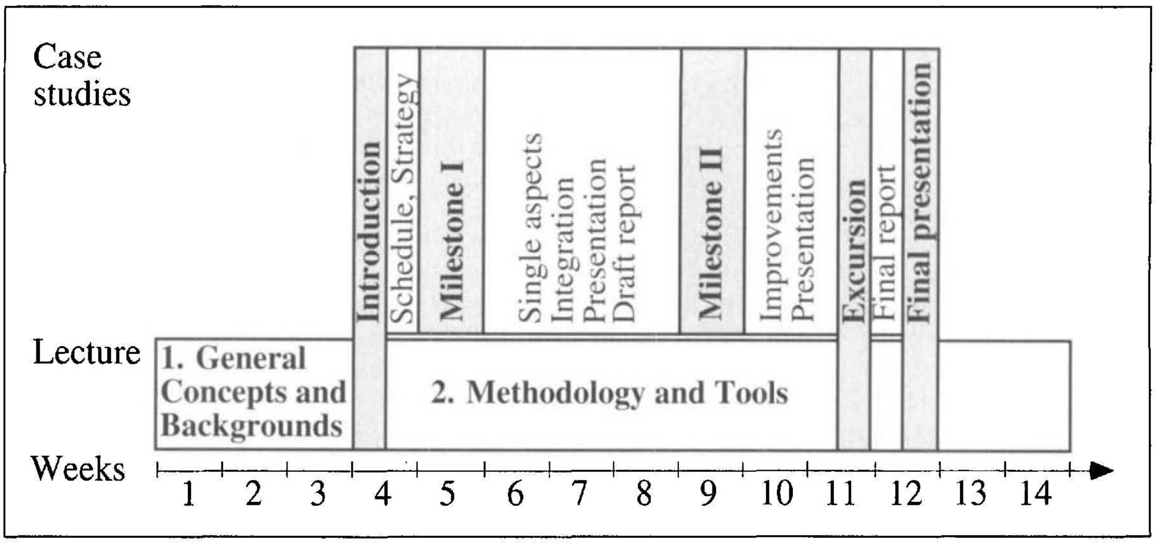

Figure. *Schedule of the case-study program*

farmers. The higher and more durable activity compensates part of the cost. However, efforts still have to be undertaken to make customers aware of the advantages of a product with a specific mode of action and with higher costs but higher activity. The chemical firms and especially their sales divisions are given the responsibility of adjusting the product's price to the financial possibilities of third-world countries and of ensuring the safe application of the insecticide.

Cases Study 2: Reactive Dyes

Reactive dyes bond covalently with textiles. They contribute annually about 15% to the overall sales revenue of textile dyes, which is equal to the production of 95,000 t per year. The new Cibachron-LS is a reactive dye used for cotton. The innovation of Cibachron-LS is that in the dying process only a quarter of the 'normal' amount of NaCl is necessary. This means a significant reduction for the ecological impact on surface water. Additionally, Cibachron-LS shows an improved performance in terms of levelness and reproducibility, resulting in enhanced process safety for the dying of cotton [5].

Case Study 3: Red Pigment

Pigments are practically insoluble, organic or inorganic coloring matter. At the beginning of the 1980s, red pigments like perylene were very common on the market. But they were not satisfactory in terms of saturation and weather resistance. Furthermore, complex multistep reaction pathways were necessary and the yields were not optimal. The new pigment 'Diketo-Pyrrolo-Pyrrole' shows significant improvements in reaction yield, simplicity of pathway, and finally in ecological and economic considerations [6].

Case Study 4: Dry Cleaning

Case study 4 was developed using a new format. The students had to suggest new strategies for the activity 'dry cleaning', rather than having to compare two products or processes. The case-study centers around the use of perchloroethylene (PER) as a dry-cleaning solvent. Consumers and environmental organizations oppose the future use of PER due to its environmental impacts. The students, placed in the role of representatives of the management of a large PER manufacturer, were given the task of evaluating new strategies and suggesting alternatives for PER. The goal of the case study was not to solve problems, but to ask the appropriate questions and to highlight critical aspects. The actual life cycle of the service 'dry cleaning' had to be analyzed and reviewed for alternative solvents, new technologies, distributions strategies, emission reduction, and recycling. Additionally, the students had to evaluate their suggestions from the points of view of society, the economy, and ecology [7].

4. Organizational Aspects of the Case Studies

Organization

The students' tight schedules at this stage in their degree courses placed strict requirements on the case-study program (*Fig.*). After three weeks of lectures about general concepts and backgrounds, the students were introduced to the case studies. An information sheet about the various case studies was distributed. One week later, the students formed about four self-selected teams of 5–6 students for each case study (totally about 80 students). For optimizing the transfer of knowledge between the different disciplines, one limitation was placed on the teams: the students from chemical engineering, chemistry, and environmental science had to be equally distributed among all teams. Each team was guided by the teaching assistant who had prepared the case study.

One week after the introduction of the case, the teams arranged the first meeting with their teaching assistant (Milestone I, 1 h). In Milestone I, the students had to present their working schedule and strategy. Questions and problems about the subject were discussed and clarified. Furthermore, each team designated a student who was responsible for the presentation of their final results.

The students worked intensively on the case studies for three weeks. They had to gather and discuss suggestions for solutions in their team and integrate the single aspects to produce a comprehensive evaluation of the products and processes. Finally, they had to plan their presentation of the overall results and produce a draft of the final report. The latter consisted of 6–10 pages containing their working strategy, results of single problems and their integration, conclusions, outlook, unsolved topics, and experiences from the teamwork. The draft of the final report had to be handed in prior to the second meeting with the teaching assistant (Milestone II, 2 h).

During the Milestone II, the contents of the draft report were reviewed, the team's results discussed and the remaining questions clarified. The goal of the second meeting was not to identify 'wrong' answers, but to encourage each team to critically review their results and to point out alternative solutions or outcomes.

During the two weeks after Milestone II, the students improved the evaluations and prepared the presentation of their results for the excursions to the chemical companies. Each excursion included not

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only the presentation of the evaluations to the professionals from the chemical companies, but also a visit to the plants where the processes were carried out. The interactive exchange of the students' results and the experience of industrial professionals was particularly valuable for the overall outcome of the case-study program. Students had the opportunity to defend their results in front of industrial experts, and at the same time they received valuable feedback about how industrials approach such problems.

In the last phase of one week, the students completed their final report, taking into consideration what they had learned on the excursion. In the last lecture parallel to the case-study program, the results of each case study were presented to the students who had worked on the other case studies and to the experts from academia and industry.

Resource Materials

Beside the script for the lecture [1], additional resource material was available to the students:

1) Case-study handout: the teaching assistants wrote detailed handouts about each case study of about 20 pages. The handouts contained the schedule of the case-study program, the goals, the questions to be answered, and finally a summary of all relevant facts about the products and processes of each case study. The information was gathered from both literature sources and from materials provided by the chemical companies. It was declared to be sufficient for the evaluation of the products and processes, so that the students could concentrate on the evaluation tools.
2) Scientific papers: *ca.* 2–3 important scientific publications with essential hints about the methods and tools were distributed.
3) Folder with partly confidential documents: each team had the chance to consult a folder that contained additional in-company information. None of the documents could be copied by the students.
4) References books and databases: various reference books and databases of the library containing safety-data sheet, process-design information, and toxicological and ecotoxicological data were recommended.

Software Tools

In the case-study program, the students got an introduction to software tools which support the evaluation of products and processes. For risk assessments of products and chemicals used in processes, the Uniform System for the Evaluation of Substances (USES) was applied [9]. This software tool evaluates substances based on a fate and exposure approach. It determines the distribution of chemicals in various environmental compartments and compares concentrations with the 'Predicted No Effect Concentration' on humans, animals, and ecosystems. Students applied this model to their problems and critically interpreted the resulting risk assessment.

Life-cycle assessment (LCA) served for the evaluation of continuous emissions during the life cycle of the products. As a special tool, the LCA software SimaPro [10] was introduced. Students investigated the life cycle of their product and analyzed the emission inventories with SimaPro. The resulting valuation indicators based on existing impact assessment methodologies had to be critically reviewed by the students.

Training in Presentation Techniques

The person in each team who was designated to give the presentation to the industrial professionals and other students attended a two-hour training in presentation techniques prepared by the Center for Teaching and Learning of the ETH.

Feedback

Student feedback about the lecture course and the case-study program was gathered in different ways: *1.* using the standard university teaching evaluation forms, *2.* with a separate questionnaire about the case-study program, *3.* during the discussion with the teaching assistant in Milestone II and the final presentation, and *4.* as part of the case-study report. In addition, the final exam indicated how well the students were able to carry out an integrated evaluation of products and processes.

5. Conclusions

The course and especially the case-study program described in this paper was successful in many aspects. First, it offered a challenge to undergraduates in chemical engineering, chemistry and environmental science to apply theory to real world problems. Second, it promoted collaboration and teamwork within the various disciplines. Third, it opened up the students' view of safety and environmental protection in a new proactive direction by a risk-oriented design of chemical technology. The final reports showed that students had expanded their previous knowledge through the application of concepts associated with integrated product and process development. Fourth, students had the opportunity to present their results and discuss their ideas with professionals from industry.

After this course, students are armed with new technical knowledge and are better prepared to work in industry and to tackle problems requiring respect for environmental, economic, and societal issues.

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