Mathematical Models in Chemistry Lessons

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Abstract
In chemistry it is often necessary to apply mathematical terms, methods and scientific paradigms in order to explain chemical phenomena. Considering the acquisition of problem solving skills in chemistry, it seems reasonable to introduce tasks, which aim at problem solving by using mathematical models. A conscious handling of mathematical models demands the transfer and usage of mathematical knowledge in new and significant situations and thus can support the comprehension of the terms that were modeled and foster problem solving skills [1]. However, it is known that students have difficulties with connecting aspects of mathematics with chemistry [2].

Since there is only rarely reliable information available from research at the moment, we researched to what extent mathematical models are actually implemented in German chemistry lessons at all and in which ways this is done. In order to investigate in which contexts mathematics should be used in chemistry lessons, the current curricula of upper secondary chemistry of all German federal states have been analysed in a first step. Based on the results of this analysis, additional approaches have been developed and carried out to get a multidimensional insight into how such issues are actually taught in everyday chemistry lessons.

In order analyse the students’ problems with using and finding mathematical models in detail, we carried out a video study (N=20) in which pupils have to work on a task of mathematical modelling in a laboratory situation with incremental learning aids.

Framework
Using mathematical models like equations, functions, graphs or geometric figures in chemistry means describing facts and data by using mathematical terms, methods or tools. Today, there are two ways of using mathematical models in chemistry lessons. On the one hand, mathematical models are used when calculating and applicating, which means finding results by using given mathematical models. On the other hand mathematical models can be created by the learners and used in a process of explaining facts and data in order to solve a chemical problem or to answer a chemical question. This process constitutes the so-called mathematical modelling.

Unfortunately, it is known that students have difficulties with connecting aspects of mathematics with chemistry [3], and teachers might be deterred from using mathematics in chemistry lessons due to those problems. However, considering the acquisition of problem solving skills in chemistry, it seems reasonable to introduce tasks, which aim at problem solving by using mathematical models. A conscious handling of mathematical models demands the transfer and usage of mathematical knowledge in new and significant situations and thus can support the comprehension of the terms that were modelled and foster problem solving skills [4].

The process of mathematical modelling can be described by a model according to Blum and Leiß (2006), which helps explaining teaching-, learning-, and thinking-processes [5,6]. Adapting this model to the process of mathematical modelling in chemistry lessons, leads to the following model [7].
Going through the process means starting with a situation in the real world. Pupils have to construct and to understand the problem or task and they have to simplify and to structure the problem in order to obtain a chemical model, such as reaction equations, laws, and resultants of chemistry. In the next step, pupils have to choose mathematical terms or methods in order to describe the problem mathematically and to obtain a mathematical model, e.g. a function or an equation. In step 4, being in the world of mathematics, pupils have to calculate to get mathematical results. Afterwards, they have to translate these results from a chemical point of view and they have to ask themselves whether these results are useful or not. Finally, they have to relate their results to the real situation.

The detailed description of the process of mathematical modelling allows a classification of students’ difficulties with mathematical modelling. More precisely, it becomes possible to specify at which individual steps in the modelling process students face problems and which consequences this might have on understanding chemical phenomena. A precondition for that is to know, where and how mathematical models shall be used in chemistry lessons according to the curricula of the German federal states and where and how they are really used in everyday chemistry lessons. Up to now, there is rarely reliable information available from research to what extent and in which ways mathematical models are actually implemented in chemistry lessons. This leads to the following research questions:

1. In which contexts should mathematics be used in chemistry lessons according to the curriculum?
2. How are mathematical models actually taught in chemistry lessons?

**Methodology**

1. In order to identify in which contexts mathematical modelling should be taught in chemistry lessons, the current curricula of upper secondary chemistry of the 16 federal states of Germany have been analysed.

2. The following approaches were chosen to provide a multidimensional insight into how such issues are taught in everyday chemistry lessons:
   - An inspection of different textbooks (N=5) served to get more details about the way the curricular guidelines are interpreted with respect to the mathematization of chemical concepts. Herein, we examined book chapters of 7 subject areas, which aim at using mathematical models according to the analysis of the curricula. All in all, we analysed 164 subchapters with their introductory texts, derivations of mathematical models and examples as well as a total of 1520 exercises.
Additionally, a qualitative analysis of the tasks of the centralised final exams for the subject chemistry has been done. It is assumed that these tasks and their sample solutions reflect which subject areas are currently deployed in chemistry lessons in secondary education and which role mathematical models play in these contexts. In this part, we analysed 31 exams (698 single tasks) of 5 selected federal states (2008-2011) in total. The selection is based on the analysis of the curricula of upper secondary chemistry (see 1).

As another part of the study, chemistry teachers (N=13) were interviewed in order to determine how the use of mathematical models is actually taught in current German chemistry lessons. Based on the knowledge about where mathematical models shall be used in chemistry lessons, we asked the teachers how they usually teach these topics.

Selected results

By analysing the current curricula of upper secondary chemistry, topics were identified, which rely on a mathematization of chemical issues. The comparison of the curricular guidelines of the 16 federal states of Germany indicated that these guidelines differ enormously:

a. The curricula of the single federal states differ in respect of the topics in which a mathematical analysis of chemical phenomena is required. For instance, half of all states request a quantitative analysis of an organic compound according to Liebig / Meyer, while the other half does not demand this topic.

b. The curricula of the single federal states differ in respect of the depth of mathematization, in particular:
   - Mathematical views are more extensive in advanced courses than in basic courses in all federal states. For example, the Henderson-Hasselbalch equation has to be taught only in advanced courses but not in basic courses in almost every federal state of Germany.
   - The curricula differ in the recommendations of how mathematical models should be implemented in class. For example, one keyword that can be found in all curricula is “the law of mass action”. However, only in few curricula the derivation of that mathematical model is explicitly recommended. This means that dealing with the law of mass action is mandatory while the derivation is not.

A closer look at the identified points, where a mathematization of a chemical topic is possible, indicates that in 32.8% of all these points an explicit recommendation of how it should be taught is included. In 82.8% a calculation or numeric example is demanded and only in 17.2% a derivation is mandatory.

Overall, two different types of using mathematics in chemistry lessons in the current German curricula of upper secondary chemistry can be identified:

- Calculating and applicating, which means finding results by using given mathematical terms, methods, tools and models (such as functions, graphs, geometric figures and coordinates)
- Derivations of chemical laws and resultants, which can be described mathematically by using mathematical terms, methods, tools or models.

Compared to the curricular requirement, the results of the substudies, which provide an insight into the actual situation, show that derivations of mathematical models of chemical issues hardly play any part:

Textbooks

The analysis of different textbooks (N=4) shows that out of 1520 exercises of those book chapters, which aim at using mathematical models, 884 exercises include a mathematical part. 99.6% of these 884 exercises demand exclusively the use of given mathematical models and only 0.4% require a derivation.

In order to describe the way of using mathematical models in tasks, the modelling process (see Fig. 1) can be used as category framework. Considering the needed single steps of the modelling process in
the tasks of the textbooks, we find that the tasks mainly deal with translating between chemistry and mathematics back and forth as well as working mathematically. Finding and validating chemical models is rarely asked in the textbooks. The following figure shows the comparison of the single textbooks with respect to the average steps which are required to solve a task (see Fig. 3).

![Comparison of the single textbooks - required steps of the modelling process](image)

**Fig. 3. Comparison of the single textbooks – required steps of the modelling process**

**Centralised final exams**

The results of the qualitative analysis of the centralised final exams show that federal states with a comparatively high mathematical share in the curriculum tend to use more mathematical models than others in their tasks of the centralized final exams. Overall, 27.7% of the analysed tasks require using mathematical models. Using mathematical models in final exams in Germany means applying given formulas.

An analysis of the tasks of the German centralised final exams in respect to the needed steps of the modelling process shows that steps of the mathematical part are asked most of all, just as in the case of the textbook tasks. But the tasks of the final exams bear more reference to a real situation than the tasks of the textbooks. Furthermore, finding and validating chemical models is asked more often in tasks of final exams than in textbook tasks (see Fig. 4). The comparison shows that there is another kind of assignment in the final exams than in the textbooks. Differences between the tasks of the final exams in the single federal states in respect to the reference to real situations are hardly ascertainable.
Teacher interviews
The teacher interviews have shown that derivations are nearly never implemented in basic courses. In advanced courses, derivations are almost exclusively presented by the teacher. In addition, the teacher always gives examples of calculations before pupils have to calculate on their own. According to the teachers, derivations can help to foster the understanding, provided that students are good at mathematics. The fewer students from one class are good at mathematics according to the teachers’ estimation, the fewer mathematical models are used by teachers in chemistry lessons. In contrast, one of the biggest problems with mathematical models from the teachers’ point of view is that students very often lack elementary chemical knowledge, rather than mathematical basic knowledge.

Video Study
With the aforementioned results which give an insight into the current teaching situation, it is now possible to analyse the students’ problems with using and finding mathematical models in detail. In order to identify these problems with mathematical modelling, we carried out a video study (N=20). Hereby, we have got an insight into the process of creating and using mathematical models in order to answer a chemical question. Furthermore, we examined whether students are able to apply and transfer competences acquired in maths class.
In order to analyse the process of mathematical modelling, tasks with incremental / stepwise learning aids [8] are used as diagnostic tool in order to identify students’ difficulties at each step of the process of mathematical modelling. As these learning aids may be designed in respect of the single steps of the modelling process, tasks with incremental learning aids allow a clear distinction of the individual steps in the modelling process and allow to differentiate between chemical, mathematical as well as learning and procedural strategies.

References