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A Novel Modelling Process in Chemistry: Merging Biological and Mathematical Perspectives to Develop Modelling Competences

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Abstract: Models are essential in science and therefore in scientific literacy. Therefore, pupils need to attain competency in the appropriate use of models. This so-called model–methodical competence distinguishes between model competence (the conceptual part) and modelling competence (the procedural part), wherefrom a definition follows a general overview of the concept of models in this article. Based on this, modelling processes enable the promotion of the modelling competence. In this context, two established approaches mainly applied in other disciplines (biology and mathematics) and a survey among chemistry teachers and employees of chemistry education departments (N = 98) form the starting point for developing a chemistry modelling process. The article concludes with a description of the developed modelling process, which by its design, provides an opportunity to develop students' modelling competence.

Keywords: models; modelling competence; chemical education

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1. Introduction

In societies that rank science and technology as highly important, enhancing pupils' participation is becoming increasingly central to teaching and learning strategies. Scientific reasoning represents an essential part of modern society since it incorporates contemporary philosophical and empirical psychological perspectives of science [1] and thereby enhances personal, social, professional and cultural participation [2]. The following six perspectives characterize the scientific reasoning: (1) postulation, (2) deployment of experiments both to control postulation and to explore observations, (3) hypothetical construction of analogical models, (4) structuring the natural variety by comparison and taxonomy, (5) statistical analysis of regularities of populations, and historical derivation of explanations [3]. Due to the central role of models in science practice and experimental studies, models are the primary method in science and scientific reasoning [2,4]. Besides appreciating the characteristics of models, their usage also belongs to scientific literacy as well [5]. Foremost in chemistry, models are essential tools for understanding and communication [6]. The great importance of models is mainly due to the nature of chemistry as a primarily abstract discipline [7]. This aspect arises from the fact that, in addition to the real visible macroscopic perspective, chemistry must consider sub-microscopic (atoms, molecules) and representational (equations, symbols) perspectives [8,9]. These characteristics lead to difficulties in the learning process for many pupils, especially when transitioning between different perspectives [10]. In contrast to the broad acceptance and importance of models and model competency in chemistry education, practice does not appear to address this issue adequately. For example, when using models in the classroom, the focus is often on describing them instead of predicting phenomena or solving problems. Furthermore, student-centred modelling is seldom anchored in practice [11]. In addition, chemistry lessons often integrate the historically oriented development of particle models from undifferentiated over less differentiated (Shell model of atoms) to strongly differentiated models (orbital models). However, this can lead to learning difficulties [12] if pupils do not competently deal with the model concept. However, properly guided, this constant development offers potential for the acquisition of competencies in chemistry.

This article addresses this issue in several steps. We start with the theoretical foundation of models and pupils' model competences in chemistry education. Subsequently, a comparison of two modelling processes to promote the modelling competence of pupils is made. Finally, we present a blended approach for a modelling process in chemistry. The results of a survey among chemistry teachers (practice-oriented relationship to chemistry) and employees of chemistry education departments (research-oriented relationship to chemistry) support the argumentation.

2. Theoretical Foundations

2.1. The Concept of Models

Models are objects or theoretical constructs created or used by a subject for a specific purpose [13]. Certain properties of the model are associated with particular properties of the represented object [14]. Thus, models do not necessarily represent a complete picture of reality but often a specific aspect [15]. Thus, the modelling process of reality under different points of view, results in various types of models. The categorization arises, for example, from the function of the models (research model versus demonstration model, [16]) or the nature of the models (virtual vs. tangible, [17]). This article considers the following two categories in more detail as they appear in the intended chemical modelling process. Pedagogical analogical models share information with the represented object. Teachers or pupils create them to explain phenomena that are not accessible to people. One or more attributes usually dominate the structure of the model to underpin the explanation [18]. Learners generate mental models within their cognitive activity during modelling processes as mental representations to describe, explain or predict phenomena [19]. When working with models in science, they take on three different functions: models are used to describe, explain or predict chemical phenomena [20]. Models function as tools to acquire knowledge or forecasting tools. In addition, they can serve as learning aids [21] by breaking down anthropomorphic ideas, reducing complex connections, generalizing circumstances or illustrating chemical and mathematical-logical processes [13]. According to previous research, analogical models enhance scientific learning if used effectively [22]. Nevertheless, the appropriate use of models is a complex cognitive activity [23]. To master this activity successfully, pupils need to acquire so-called model competence [24].

2.2. Model Competence

Model competence used in biological contexts is the ability "to gain purposeful new insights into ... topics using models, to judge models concerning their purpose, and to reflect on the epistemological process using models" [25] (p. 55). According to the second and third lines of Table 1, model competence has two sub-dimensions: knowledge about models and modelling. 'Knowledge about models' covers the conceptual part of competence and subsumes the 'nature of models' and 'multiple models'. In the dimension 'nature of models', learners compare the model and the represented object in terms of similarities and differences. In the context of 'multiple models', reasons for the existence of different models of a specific object are discussed. 'Modelling' as the procedural part of the model competence summarises 'purpose of models', 'testing models' and 'changing models'. The purposes merged under the category 'purpose of models' are general reasons for existing models and reasons to create and apply models (e.g., construction and evaluation of experiments, justification of causal relationships). Thus 'testing models' involves integrating different perspectives into the model, whereas a hypothesis may be tested by using the model. The formulated three levels of competence for each of these sub-categories (Level I: exclusive consideration of the model; Level II: factual explanation of the phenomenon to generate understanding; Level III: hypothetical–deductive investigation of the phenomenon) allows a classification of the learners' proficiency levels [26].

Table 1. Model–methodological competence [extension of 25].

Model-Methodological Competence				
Model Competence Knowledge about Models (**Conceptual**)		**Modelling Competence** Modelling (**Procedural**)		
nature of models	multiple models	purpose of models	testing models	changing models

Here, we propose a further differentiation between model competence and modelling competence to emphasize the procedural character to a greater extent. Modelling competence is the ability to initiate a theory-guided or creative process of cognition when creating models, to gain knowledge related to purpose when using models, make judgements about models regarding their purpose, and to reflect on the process of acquiring knowledge through models and modelling [27]. Comparable to the model competence (2nd and 3rd line of Table 1), the new definition specifies the epistemological procedures into a theory-based orientation and creative development. As a result, the sub-dimensions show four competence levels each [28]:

- Level I: Exclusive consideration of the model;
- Level II: Factual explanation of the phenomenon to generate understanding;
- Level IIIA: Abductive reasoning explanation of the phenomenon;
- Level IIIB: Hypothetical-deductive investigation of the phenomenon.

Following, but not in entire agreement with this definition, this paper defines model-methodical competence as an umbrella term of modelling competence (previously called 'knowledge about models', conceptual part) and the modelling competence (previously called 'modelling', procedural part) (light green terms in Table 1). The sub-dimensions remain in their allocation in the new definition. This distinction emerges from the differentiation between practical and meta-modelling knowledge [29].

2.3. Modelling Processes

The deep rootedness of models in science education described above emphasizes the promotion of modelling competence as a central task of chemistry education [30]. Thoughtful consideration of modelling processes as iterative cycles of creating, applying and reviewing models enables competence promotion [31]. In this context, students' active manipulation of models positively affects model competence in three ways [32]: First, hands-on experience with models enables a cognitive off-load. Three-dimensional representations can spare cognitive capacities. Second, the pupils perceive multiple representations as they revise previous representations themselves or see the representations of their fellow pupils. The integration of various representations allows the learners to create more comprehensive and coherent mental models. Third, the physical confrontation with the model encounters various stimuli (such as cues from the touch) in the long-term memory, forming more bonds between the learning content and the long-term memory. This approach becomes even more critical against the background that pupils have not developed model competence in the sense mentioned above in a satisfactory way [33].

2.4. Modelling Process 1: Formally Used in Biological Contexts

The first modelling process formally used in biological contexts (Figure 1) starts with an experiment or a daily observation [34]. The data obtained on this basis influence the following preliminary considerations. Based on this, a model is generated in creative development, used to create a hypothesis. The hypothesis is then either verified or falsified by further data. In the last case, the cycle is rerun using new data until the hypothesis can finally be accepted.

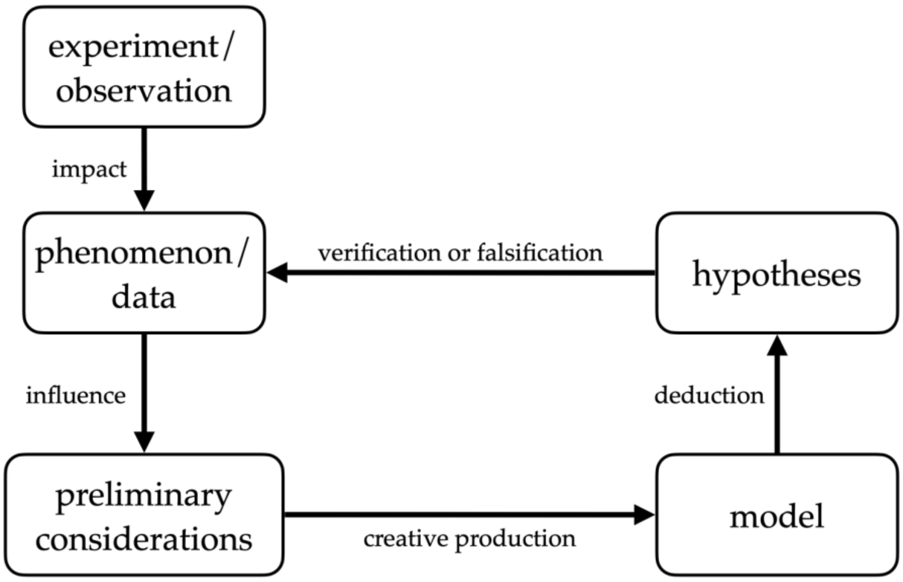

Figure 1. Scheme to promote model competence [34].

2.5. Modelling Process 2: Formally Used in Mathematical Contexts

The modelling circle shown in Figure 2 is formally used in mathematical contexts and reduced to the essentials. This process distinguishes in a 2 × 2 design between the world and mathematics as well as between the resulting problem and its mathematical solution [35]. In the chemical context of modelling, mathematics is equal to the model world. The starting point of this modelling process is an outer-mathematical problem (situation). A mathematical model with an inner-mathematical problem is generated from the situation by (mathematical) modelling. Applying mathematical rules and procedures causes an inner-mathematical consequence from the problem. In the next step, the modeller relates the mathematical results to the real world to obtain and check the plausibility of the mathematical results. If the result is not considered a valid answer for the initial situation, the process is rerun.

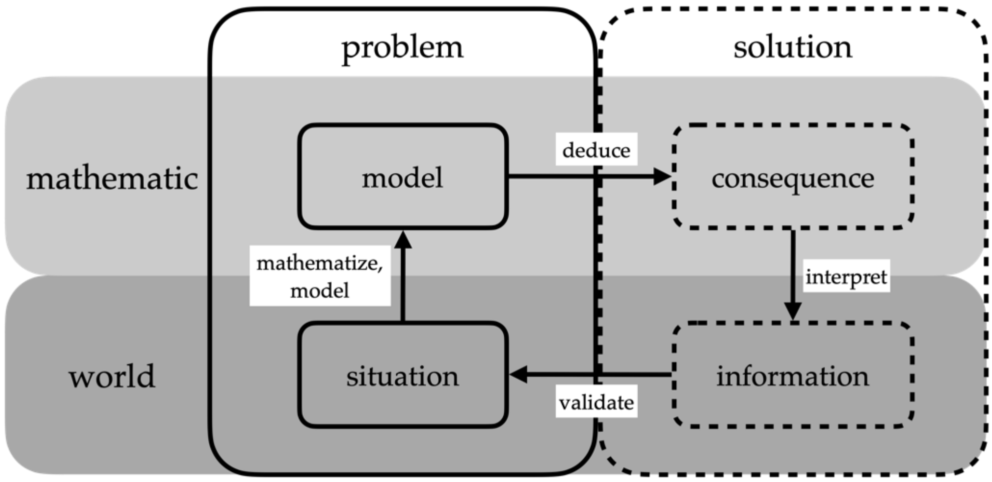

Figure 2. Mathematical modelling process [35].

3. Method

3.1. Research Questions

Based on the presented relevance of models and model competence for chemistry teaching, the online questionnaire covers the experiences with models (R 1) and model competence (R 2) of didactical experts in chemistry (chemistry teachers with a practice-oriented relationship to chemistry and employees of chemistry education departments with a research-oriented relationship to chemistry). Table 2 provides an overview of the research questions.

Table 2. Overview of the research questions.

Models in Teacher Training, Chemical Education Research or Chemistry Teaching
R 1. Which aspects related to models do anchor in teacher training, chemical education research or chemistry teaching?
Model competence
R 2a. To what extent is a well-developed model competence perceived as important for chemistry education? R 2b. To what extent do the respondents agree with the dimensions of model competence [19] (Table 1) in the chemical context?
Modelling processes
R 3a. How do the respondents assess the transferability of modelling processes from other disciplines to chemistry in general? R 3b. To what extent can the presented modelling process 1 (Figure 1) be transferred to chemistry? R 3c. To what extent can the presented modelling process 2 (Figure 2) be transferred to chemistry? R 4. Considering theoretical aspects and expert opinions, how can a novel modelling process for chemistry look like?

Modelling processes provide a method for promoting model competence [24]. These processes vary in their focus depending on the subject area (modelling processes 1 and 2 in Sections 2.4 and 2.5). Based on this, the respondents estimate to what extent approaches from other disciplines are transferable to modelling in chemistry (R 3a). Subsequently, the questionnaire presents the two modelling processes from Sections 2.4 and 2.5, and the participants precisely assess their suitability for chemistry (R 3b + c). The survey ultimately aims to design a novel chemistry modelling process that considers theoretical aspects and expert opinions (R 4).

3.2. Questionnaire

The first questions of the questionnaire collect background data. In addition to the relationship to chemistry (practice-oriented or research-oriented), this includes gender, age, teaching qualification (primary school, community school, vocational school, secondary school or other), location of study, school subjects, professional experience and research areas (for employees of chemistry education departments). Conforming to the research questions, the central part of the questionnaire consists of the sections: Models, Model competence and Modelling processes. Table 3 compiles an overview of the questions and associated answer options in the central part of the questionnaire. The questions in the Models section (Q1 to Q3, Table 3) capture the degree to which education, chemistry education research or chemistry education integrate models and which aspects they explicitly address. The subsequent part on model competence first presents the definition of model competence (Table 1). The respondents then evaluate this definition regarding its transferability to chemistry and give their subjective assessment of the importance of a strong model competence for chemistry (Q4, Table 3). Finally, the respondents name aspects of the definition that fit well for chemistry and what should be omitted, added or changed if necessary (Q5 and Q6, Table 3). The last part about modelling processes starts with a general assessment of whether the respondents could imagine transferring modelling processes from biology or mathematics to chemistry (Q7 a and b, Table 3). After a video-based presentation of the first modelling process, the participants specifically indicate how to transfer to chemistry. In three open-ended questions, respondents then identify aspects that transfer well to chemistry, modify or omit, or add to better fit chemistry modelling (Q8 and Q9, Table 3). The final questions regarding the mathematical modelling process (Figure 2) are the same as those concerning the biological modelling process before (Q10 and Q11, Table 3).

Table 3. Overview of the central part of the questionnaire.

Models

Q1. Did you get to know different models in chemistry (cf. particle models, molecule kits, model experiments) during your education?

1. *"No, I have never got to know different models in chemistry."*
2. *"Yes, during university education."*
3. *"Yes, during the second phase of training (preparatory service)."*
4. *"Yes, during in-service training or seminars."*
5. *"Yes, in the course of the following measure:" (open-ended answer)*

Q2. Do you/Does your research group explore different models in your/their research (cf. particle models, molecule kits, model experiments)? (research-orientated participants only)

1. *"No, I do not explore/ my research group does not explore different models."*
2. *"Yes, I explore different/ my research group explores models theoretically."*
3. *"Yes, I explore different/ my research group explores models practically concerning the use of different models, cf. by developing and testing possible applications for everyday school life."*
4. *"Yes, I explore different/ my research group explores different models in an inferential way:" (open-ended answer)*

Q3. In your chemistry lessons, do you employ different models (cf. particle models, molecule kits, model experiments)? (practice-orientated participants only)

1. *"No, I do not employ models in my lessons."*
2. *"Yes, I employ theoretical models (cf. particle models) in my lessons."*
3. *"Yes, I employ analogue models (cf. molecule kits) in my lessons."*
4. *"Yes, I employ conceptual models in my lessons (cf. mental representations of chemical laws such as the law of conservation of mass) to make and check predictions."*
5. *"Yes, I employ model experiments in my lessons (cf. Stechheber experiment)."*
6. *"Yes, I employ models in my lessons as follows:" (open-ended answer)*

Model competence

Definition of Model competence (Table 1)

Q4. Please indicate how much you think the following statements are true.

(a) "For me, this definition of model competence applies just as well to chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree'.*

(b) "For me, I see a well-developed model competence of the students according to the definition mentioned above as very important for chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree.*

Q5. Which of the above aspects would you apply to model competence in chemistry?
open-ended answer

Q6. Which aspects would you modify, add or omit for better applicability to model competence in chemistry?
open-ended answer

Modelling processes

Q7. Please indicate how much you think the following statements are true.

(a) "In my opinion, modelling processes from biology are good transferrable to chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree.*

(b) "In my opinion, modelling processes from mathematics are good transfer-rable to chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree.*

Table 3. *Cont.*

Models
Video-based presentation of Modelling process 1
Q8. Please indicate how much you think the following statements are true. "In my opinion, modelling processes from biology are good transferrable to chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree.*
Q9. Which aspects of the modelling process from biology . . . (a) " . . . fit well and are adaptable for chemistry, in your opinion?" *open-ended answer* (b) "... do not fit well and should be modified or omitted for chemistry, in your opinion?" *open-ended answer* (c) "... in your opinion would have to be supplemented for the scheme to repres-ent a modelling process in chemistry?" *open-ended answer*
Video-based presentation of Modelling process 2
Q10. Please indicate how much you think the following statements are true. "In my opinion, modelling processes from mathematics are good transferrable to chemistry." *4-point Likert scale ranging from 1 'disagree' to 4 'agree.*
Q11. Which aspects of the modelling process from mathematics . . . (a) " . . . fit well and are adaptable for chemistry, in your opinion?" *open-ended answer* (b) "... do not fit well and should be modified or omitted for chemistry, in your opinion?" *open-ended answer* (c) "... in your opinion would have to be supplemented for the scheme to represent a modelling process in chemistry?" *open-ended answer*

3.3. Participants

A total of 98 participants completed the qualitative questionnaires via Unipark. Among them, 56 (57%) were completed by research-orientated people (University) and 42 (43%) by practice-orientated people (School), with a total of 44 (44,9%) female, and 52 (53,1%) male (2 abstentions). The mean age amounts to 40.18 years (SD = 14.76), and 78 out of 98 (80%) respondents hold secondary school teaching qualifications. The most common teaching subject besides chemistry is biology (37 out of 93, 38%). Among the research-oriented participants, the number of people without professional experience of teaching at school is high (25 out of 56, 45%). In comparison, this proportion is only 17% (7 out of 42) among the practice-oriented participants. Table 4 shows an overview of the background data.

Table 4. Background data of the survey.

	In Total (*n* = 98)	**Research-Orientated Relationship (*n* = 56)**	**Practice-Orientated Relationship (*n* = 42)**
Gender	m = 52; f = 44	m = 31; f = 23	m = 21; f = 21
Age	M = 40.18; SD = 14.8	M = 39.02; SD = 15.5	M = 41.75; SD = 13.7
Teaching qualification	ps = 4; cs = 6; vs. = 2; ss = 78; o = 8	ps = 2; cs = 4; vs. = 2; ss = 43; o = 5	ps = 2; cs = 2; vs. = 0; ss = 35; o = 3
Location of study	bw = 9; by = 11; b = 5; bb = 1; hh = 1; he = 5; mv = 2; *n* = 5; nrw = 20; rlp = 5; sl = 18; s = 1; sa = 1; sh = 4; t = 3; o = 3	bw = 3; by = 9; b = 4; he = 4; mv = 1; *n* = 4; nrw = 15; rlp = 3; sl = 1; s = 1; sa = 1; sh = 3; t = 3; o = 2	bw = 6; by = 2; b = 1; bb = 1; hh = 1; he = 1; mv = 1; *n* = 1; nrw = 5; rlp = 2; sl = 17; sh = 1; o = 1
School subjects (selection)	biology = 35 mathematics = 18 physics = 11 Science = 8	biology = 19 mathematics = 8 physics = 8 Science = 3	biology = 16 mathematics = 10 physics = 3 Science = 5

Table 4. *Cont.*

	In Total (n = 98)	Research-Orientated Relationship (n = 56)	Practice-Orientated Relationship (n = 42)
Professional experience at school	M = 11.27; SD = 13.2 *(0 years: 32 of 98)*	M = 9.98; SD = 14.7 *(0 years: 25 of 56)*	M = 12.85; SD = 11.2 *(0 years: 7 of 42)*
Research Area (selection) n = 56	X	Digitalization = 20 Teacher education = 16 Experiments = 15 Models = 10	X

Key: m, male; f, female; ps, primary school; cs, community school; vs, vocational school; ss, secondary school; o, others; bw, Baden–Württemberg; by, Bayern; b, Berlin; bb, Brandenburg; hb, Bremen; hh, Hamburg; he, Hessen; mv, Mecklenburg–Vorpommern; *n*, Niedersachsen; nrw, Nordrhein–Westfahlen; rlp, Rheinland–Pfalz; sl, Saarland; s, Sachsen; sa, Sachsen–Anhalt; sh, Schleswig–Holstein; t, Thüringen.

4. Results

4.1. Models

In the first section of the survey, the participants state that they all had experience of various models and mostly during their university education (72 out of 98; A in Figure 3). The chemistry education research models are rarely present, while theoretical and practical research approaches are approximately equally widespread (26 and 24 out of 56; B in Figure 3). In chemistry lessons, all the participants reported that they implement models in their teaching. Theoretical models occur to the same extent as analogue models (40 out of 42, 95.3%). Nevertheless, the teachers also use conceptual models (36 out of 42) and model experiments (34 out of 42, C in Figure 3).

4.2. Model Competence

Concerning model competence, the respondents not only considered model competence to be important for chemistry (MD = 3.40 of 4), but also could imagine transferring the model competence dimensions to their work (MD = 3.37 of 4; D & E in Figure 3). Most participants agreed that all the aspects to apply to chemistry (58 out of 98, F in Figure 3). The 'nature of models' was seen as critical for chemistry by 14 out of 98 people, with six participants with a research background stating the reason for this was that the initial object in chemistry is not empirical compared to objects in biology. These statements are consistent with the fact that in chemistry, frequently used models are models themselves, objects may be directly employed [10]. For example, chemists apply atomic models to explain macroscopic phenomena, mainly because the atomic structure is not observable directly. Therefore, modelling in chemistry operates on a different level. Furthermore, eight out of 98 respondents criticized the sub-dimension 'multiple models' with the explanation of a low significance of this dimension in the chemistry classroom (Q6, Table 5). Certain participants suggested adding types of models to the sub-dimension 'nature of models' or renaming 'changing models' to 'expanding models'. These results indicate that this competence definition is suitable for chemistry, but also that certain refinements are necessary.

4.3. Modelling Processes

In the previous section on modelling processes, the respondents rated the transferability of the modelling processes as neutral (2.85 (biology) and 2.58 (mathematics) on a 4-point Likert scale ranging from 1 'disagree' to 4 'agree'; G & H, Figure 3). After a video-based introduction of the modelling process formally used in biological contexts, the respondents rate the transferability of this process as rather good (M = 3.27 of 4; SD = 1.1; I in Figure 3). The participants indicated in open formats which aspects of the process fit well, which work more poorly and what the participants would probably like to add (Q9 a, Table 5). 61% (47 out of 77) agreed with all of the aspects, while 14 of 77 (18%) positively highlighted the experiment and 11 of 77 (14%) the formation of a hypothesis.

28 out of 65 (43%; Q9 b, Table 5) could not identify any aspect that should be changed or omitted in their opinion, though 6 out of 65 (9%) were critical of 'creative production'. One criticism was, for example, that other aspects (cf. available resources) influence the 'creative production' besides the preliminary considerations. Concerning supplements, 14 out of 60 (23%) did not indicate anything (Q9 c, Table 5), while 10 out of 60 (17%) would like to add different levels of representation. This requirement matches the literature [8,36]. The second modelling process formally used in mathematical contexts takes this into account.

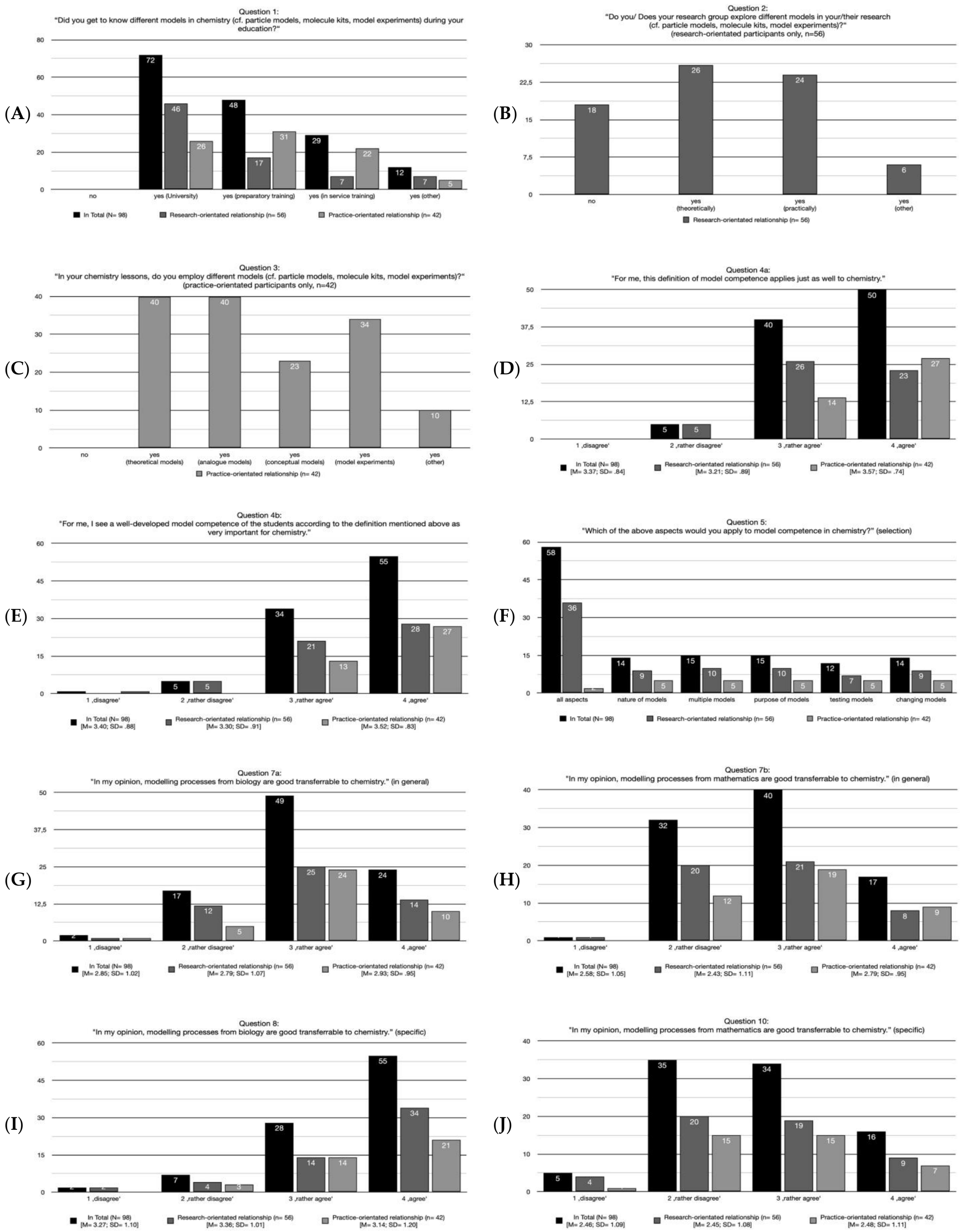

Figure 3. Results of the closed-ended questions. Diagrams showing the results of (**A**) question 1, (**B**) question 2, (**C**) question 3, (**D**) question 4a, (**E**) question 4b, (**F**) question 5, (**G**) question 7a, (**H**) question 7b, (**I**) question 8 and (**J**) question 10.

Table 5. Results of the open-ended questions.

Questions According to Table 3	In Total (N = 98)	Research-Orientated Relationship (n = 56)	Practice-Orientated Relationship (n = 42)
Model competence			
Q6 (selection)	n = 14; m = 8; p = 3; t = 7; c = 7	n = 11; m = 5; p = 3; t = 6; c = 3 "initial object unknown in chemistry" = 6 "Add types of models" = 2	n = 3; m = 3; p = 0; t = 1; c = 4 "rename 'changing models' to 'expanding' models" = 2
Modelling Processes			
Q9 (selection)	(a) a = 47; e = 14; h = 11; c = 7 (b) no = 28; pc = 6; cd = 6; m = 3; e = 4 (c) no = 14; lr = 9; e = 7; mm = 3	(a) a = 33; e = 6; h = 6; c = 3 (b) no = 17; pc = 4; cd = 4; m = 3 (c) no = 10; lr = 5; e = 5; mm = 3	(a) a = 14; e = 8; h = 5; c = 4 (b) no = 11; pc = 2; cd = 2; e = 4 (c) no = 4; lr = 5; e = 2
Q11 (selection)	(a) a = 8; dwm = 12; v = 10; m = 6; co = 6 (b) a = 2; no = 2; ma = 11; clr = 4 (c) no = 4; amp1 = 22; bm = 2	(a) a = 6; dwm = 10; v = 7; m = 6 (b) a = 2; no = 2; ma = 7 (c) no = 2; amp1 = 14; bm = 2	(a) a = 2; dwm = 2; v = 3; co = 6 (b) ma = 4; lr = 4 (c) no = 2; amp1 = 8

Key: Q9: a, all; e, experiment; h, hypotheses; c, cycle; no, nothing; pc, preliminary considerations; cd, creative development; m, models; lr, levels of representation; mm, mathematical models. Q11: a, all; dwm, distinction between the world and mathematics; v, validation; m, modelling; co, consequence; no, nothing; ma, mathematization; de, deduction; i, interpretation; lr, levels of representation; amp1: aspects of modelling process 1; bm, blended model.

The structure of this part of the questionnaire is analogous to the first modelling process: at the beginning, a video represents the process to the participants. Afterwards, they rate the transferability of this process as neutral (M = 2.46 of 4; SD = 1.1; J in Figure 3). The respondents were asked subsequently in an open form to indicate aspects that fit well, fit poorly and elements that probably need to be supplemented (Q11 a to c, Table 5). Eight out of 70 (11%) respondents saw all aspects as transferable to chemistry, while 17% (12 out of 70) perceived the juxtaposition of the 'world' and 'mathematics' (model world) as highly effective. Another 10 out of 70 (14%) highlighted referring to the real situation ('validate') as positive. The validating step aligns with the general orientation of chemical education towards everyday phenomena (cf. the processing circuit of chemistry in context, [37]). Significantly few participants (2 out of 56, 4%) stated that they would not change the presented aspects. Eleven of 56 (20%) named 'mathematize' as needing change, as mathematization rarely matters in the chemical modelling process. Among the supplementary proposals, 20 out of 55 participants (37%, Q11 in Table 5) mention aspects of the biological approach. These are copying effects created by the order of the tasks [38]. Apart from that, the participants named several different aspects. However, these only occurred twice each: The process makes sense if there is a transition between macroscopic and sub-microscopic levels, which is not the case in every chemical modelling. There should be an experiment or theoretical basement integrated as the starting point, which takes the importance of the experiment as the second central method of science into account [2].

4.4. Suggestion for a Novel Modelling Process in Chemistry

- The following consequences for modelling in chemistry emerge from the previous explanations:
- The aspects of the first modelling process (Figure 1) generally remain unchanged;
- The second model (Figure 2) emerges that the process needs to differentiate between the macroscopic real world and the sub-microscopic modelled world;
- For clarifying the cognitive processes (cf. mental analogue models), a separation occurs between perceptual and non-perceptual modelling steps;

- The modelling process should integrate phases to improve model-methodical competencies at appropriate points.

The developed process for modelling in chemistry shown in Figure 4 distinguishes between two different levels: the real macroscopic and the sub-microscopic modelled level. This explicit separation enables the pupils to consciously switch between the macro and sub-micro worlds with their unique peculiarities and regularities. The modelling process starts with a phenomenon that pupils can observe in their everyday lives. This starting point considers the general didactic demand for relevance in chemistry lessons [39]. Conversely, it enables students to understand that they should develop a model [40]. The experiment or phenomenon provides (experimental) data or observations that depend strongly on personal factors (e.g., disciplinary knowledge, theories, attention, [41]). In the following step, the modeller activates their prior knowledge and conceptual model competence (sub-categories 'nature of models' and 'multiple models', cf. *n* and M in Figure 4) to form a mental model. Here, a transition takes place in two ways. There is a change from the experiential real world to the model world (in Figure 4: light grey or dark grey background). Conversely, visible (Figure 4: solid outlines) processes become invisible (Figure 4: dashed contours). Using inner (modelling competence, creativity) and outer resources (learning situation, available materials), the modeller generates an analogue representation out of the mental model, a so-called pedagogical analogical model [19]. Mental models are simply a stopover in forming an analogical model. Nonetheless, the discrepancy is essential in analysing pupils' concepts because mental models and their analogous representations do not necessarily coincide. The analogical model subsequently allows hypothesis generation. In this step, the model world refers to reality, i.e., the learner must once again make a 'world transition'. This step gives pupils an understanding of the competence dimension' purpose of models'. Within the macroscopic world, the pupils generate experimental settings or everyday phenomena that provide observations or data to verify or falsify the hypothesis. By testing the hypothesis, learners create a reference to the modelling competence dimension 'testing models'. In the case of a falsified hypothesis, the modellers go through the cycle again. First, they change their mental model and thus also the analogical model. Through the model modification, the modelling process establishes a relationship to the competence 'changing models'.

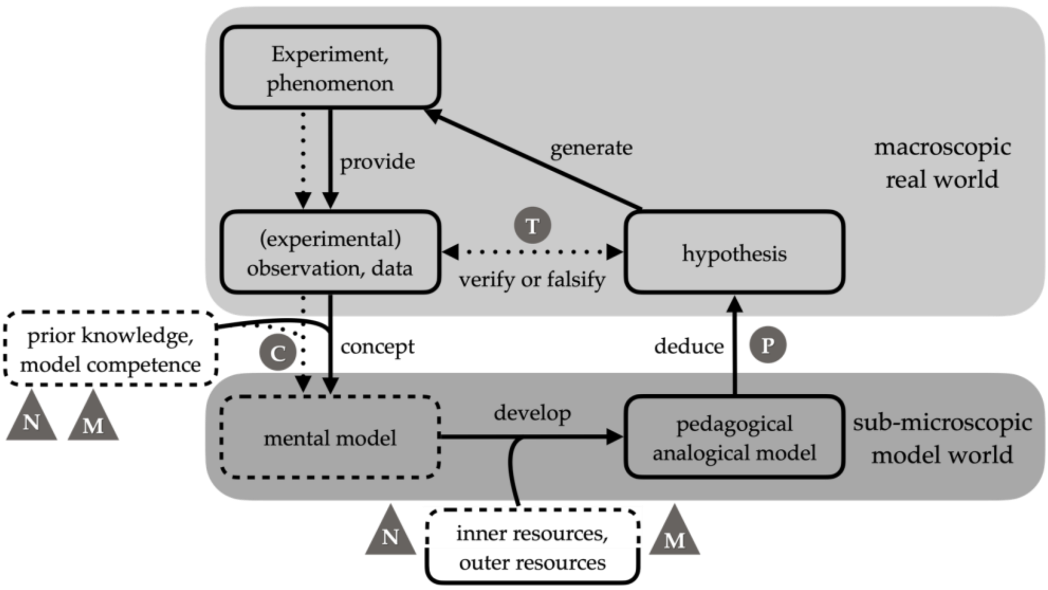

Figure 4. Modelling process in chemistry to promote modelling competence. Notice: The icons mark points to address the sub-competencies during the process (round icons)/applied (triangular icons) (N, nature, M, multiple, P, purpose, T, testing, C, changing).

A hypothetical example from school practice on states of matter serves to concretize the proposed modelling process for chemistry (Figure 5). The pupils observe the evaporation of water in their everyday life, for example, when cooking. From this, they derive data, the boiling temperature of the water or the optical properties of water vapour, for example. To explain these data, the pupils activate their prior knowledge of the undifferentiated particle model and their model competence. This activation generates a pictorial representation in the students' minds–a mental model (pictorial mental representation in Figure 5). Using coloured cardboard or other craft materials, the pupils visualize their mental representation to form a pedagogical analogue model (visualization in Figure 5). For example, circles cut out from cardboard could be arranged at small distances to represent the liquid state and at large distances for the gaseous state. In this step, personal skills (creativity, manual skills) play an essential role. The analogue model is now observable for the teacher and the fellow pupils. From the analogue model, the students then derive, for example, the hypothesis that a certain amount of substance would have to occupy a larger volume after the transition from the liquid to the gaseous state of matter since the movement of the particles increases and the particles occupy the entire available volume. To test the hypothesis, the students then perform the experiment on the evaporation of acetone to exemplify the transitions between the states of matter in a closed system (pointed arrows in Figure 5). They place a few millilitres of acetone into a plastic bag and close it airlessly. Using a hot water bath, the students then heat the acetone and see that the bag inflates. The hypothesis can therefore be accepted, which strengthens the students' model conception.

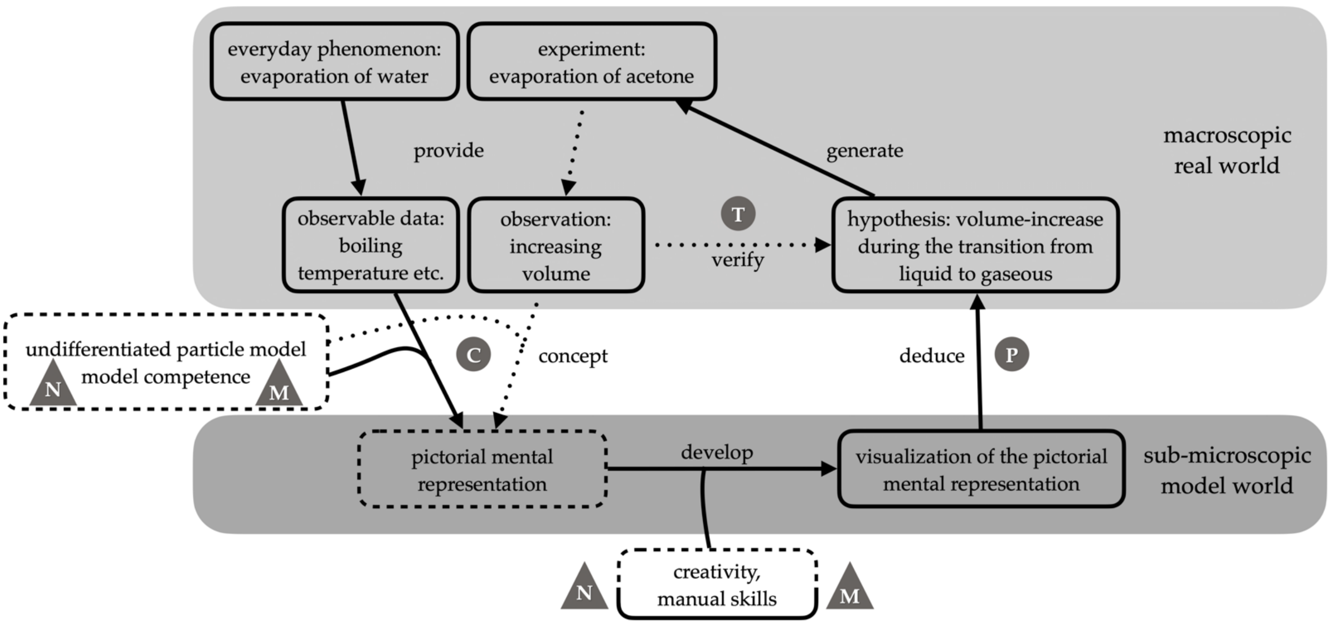

Figure 5. Hypothetical example of the modelling process in chemistry from school practice. Notice: The icons mark points to address the sub-competencies during the process (round icons)/applied (triangular icons) (N, nature, M, multiple, P, purpose, T, testing, C, changing).

5. Discussion

The following section discusses the developed model on the basis of accepted didactic concepts and classifies the idea correspondingly. In the SDDS approach, Klahr & Dunbar [42] anchor modelling in scientific reasoning. The approaches of Clement [43] and Göhner & Krell [44] support the basic structure. The basic structure consisting of conjecture, evaluation and modification or reflection of Clement [43] and Göhner and Krell [44] is common to the developed scheme. In addition, loops are integrated in all approaches, enabling a reference back to the question, hypothesis or built model. The developed scheme of a modelling process agrees with Göhner and Krell [44] in the distinction between the macroscopic real world and the sub-microscopic model world. In this context, Steinbuch [45] describes that with every transition between the real and the model world, filtering always occurs, in which the subject only processes aspects that are considered important. Moreover, the developed model additionally distinguishes between observable and non-observable stages according to Harrison and Treagust's [18]. Fratiwi et al. additionally emphasise the importance of knowing students' mental models in order to assess their scientific understanding [46]. Therefore, the scheme includes mental models as well as analogue models. Mental models and formed analogue models often differ and consequently, the captured modelling competence can differ from the actual modelling competence. Moreover, Didiş, Eryılmaz and Erkoç [47] describe the basis for the formation of mental models as a combination of scientific and non-scientific fragments, whereby the developed schema incorporates prior knowledge and model competence. When creating the analogue model, the influencing factors (model competence, prior knowledge, external and internal resources) are again considered. Above this, the focus of the second part of the scheme (formation of hypotheses and seeking of verification or falsification) bases on the separation between search hypothesis space, test hypothesis and evidence evaluation of the SDDS approach [42]. At last, the novel scheme, based on the reflection scheme of Caspari et al. [48], establishes relationships to the competence dimensions at the appropriate points to force the promotion of modelling competence.

6. Conclusions

The blended process presented here brings the positive aspects of both modelling cycles together and compares them with the expert opinions from the survey. The design of an intervention will rest on this such that it is suitable for promoting modelling competence. The process will consider the complexity of modelling [23] and the pupils' attitudes by supporting them individually in their learning [49]. Unlike other studies that locate modelling processes in the upper secondary school [48,50], the intervention is anchored in initial chemistry teaching. Research has shown that misconceptions are stable over time and difficult to correct, including with increasing subject knowledge [51]. Nevertheless, the cognitive abilities of pupils increase during their school career, which means that the complexity of modelling processes can also rise to increase educational attainment [10]. Therefore, a spiral curricular promotion of modelling competence is apparent and suggested in the survey responses.

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