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Tracking student learning across a conceptual landscape: transitions and differential changes in conceptual modes during a unit on chemical kinetics and equilibrium

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Understanding chemical reactions (CR) is central to both disciplinary learning and informed engagement with societal issues in which content knowledge about CR is relevant. While prior research has mapped students' conceptual development in CR during lower secondary education, little is known about students' progression during upper secondary levels, particularly in response to targeted instruction. This study investigates how students' conceptual modes – specific reasoning patterns about the start, progress, and end of chemical reactions – develop following instruction on chemical kinetics and chemical equilibrium. Drawing on a pre–post study conducted over an extended instructional period, we assessed N = 183 German upper secondary students' conceptual understanding using open-ended tasks before and after participation in a digitally implemented teaching unit. Conceptual modes were analyzed both descriptively and inferentially, incorporating difference-in-differences estimation and ordinal logistic regression to examine instructional effects and the role of prior knowledge. We included subject-related interest as an exploratory covariate. Results show significant transitions towards more sophisticated mechanistic reasoning, particularly among students who received instruction on both kinetics and equilibrium. Prior conceptual modes emerged as a strong predictor of post-instruction understanding, highlighting the cumulative nature of conceptual development as well as the diagnostic potential associated with this approach. We discuss implications for designing learning environments that scaffold mechanistic reasoning in chemistry and support the continuity of learning progressions across educational stages.

Introduction

Understanding chemical reactions is not only relevant for academic or professional pathways in chemistry but also plays a key role in preparing learners to engage with complex scientific issues such as energy transitions and environmental challenges (Anastas and Warner, 1998; Scharf and List, 2022; Schettel, 2022). In order to support learners in building up disciplinary core concepts that enable both knowledge acquisition as a basis for cumulative content learning and meaningful, contextualized application, such as engaging in informed discussions of societal relevance (Parchmann *et al.*, 2006; Childs *et al.*, 2015), chemical understanding needs to be developed progressively across educational stages. Approaches like learning progressions (Duncan and Hmelo-Silver, 2009) commonly suggest a spiral-curricular organization of knowledge where learners revisit core ideas with increasing depth and sophistication. One such core idea is the concept of chemical reactions (CR), which underlies key aspects of chemical reasoning and practice, including transformation, analysis, and synthesis (Sevian and Talanquer, 2014). Although cross-sectional studies have demonstrated cumulative development in students' understanding of chemical reactions over time (Boo and Watson, 2001; Yan and Talanquer, 2015; Emden *et al.*, 2018), they also reveal persistent difficulties in developing a process-oriented understanding of chemical change – an understanding that is crucial for engaging with energetic and environmental issues in a competent way. Mastery of CR involves a highly interconnected knowledge structure and poses significant conceptual challenges, even at the secondary level (Van Driel *et al.*, 1998). Nonetheless, such mastery is foundational for future learning in related content areas (*e.g.*, Edelsbrunner *et al.*, 2024). While this underscores the importance of connectable conceptual knowledge, systematic research on the development of students' understanding of chemical reactions is relatively well established at the lower secondary education level but remains sparse concerning the transition to and progression within upper secondary education. This phase of education, which bridges school and university-level chemistry, plays a crucial role in shaping learners' conceptual

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trajectories. Yet, to the best of our knowledge, existing studies have been predominantly cross-sectional in design and have thus failed to capture within-person development. The aim of this study is therefore to examine how upper secondary students' understanding of chemical reactions develops over time – after several weeks of instruction on chemical kinetics and chemical equilibrium, two central topics within the core concept CR. By adopting a pre–post design over an extended instructional period, we aim to trace shifts in students' conceptual modes (Yan and Talanquer, 2015) that reflect increasingly sophisticated mechanistic reasoning. In doing so, we also examine cognitive and affective predictors of this development and identify both instructional effects and persistent conceptual challenges. These findings allow us to derive implications for the development of a learning progression for upper secondary education and for designing learning environments that foster interconnected conceptual understanding of chemical reactions.

Theoretical background

Research on chemical reactions at the lower secondary level has provided important findings, particularly through empirically validated learning progressions (LPs), which describe how students' understanding of core concepts evolves with instruction towards increasingly sophisticated ways of mastery (Corcoran *et al.*, 2009; Duncan and Hmelo-Silver, 2009). In contrast, upper secondary education has received far less systematic attention. Based on the available evidence (Yan and Talanquer, 2015), we propose a teaching–learning sequence (TLS), understood as a research-informed instructional design approach (Méheut and Psillos, 2004; Bernholt and Sevian, 2018), which informed the instructional unit in this study.

Conceptual development of students' understanding of chemical reactions

Current state of research. Many studies have focused on students' chemical understanding in a more global way with a strong focus on the particle model of matter (Krnel *et al.*, 1998; Liu, 2001; Harrison and Treagust, 2003; Johnson, 2002) or alternative conceptions (Garnett *et al.*, 1995; Talanquer, 2006). However, we would like to explicitly focus on the concept CR, since comprehensive knowledge within this core concept is essential for many typical ways of thinking and working (analysis, synthesis, transformation) in our discipline. While this need for detailed understanding also applies to other areas of chemistry, chemical reactions represent an integrative element, or a *conceptual hub*, that directly connects macroscopic, particulate, and structural-energetic aspects.

While many previous studies in relation to school learning have examined specific aspects within this core concept – *e.g.* learning difficulties (*e.g.* Akkus *et al.*, 2003), misconceptions (*e.g.* Boujaoude, 1991; Özmen and Ayas, 2003), or specific contexts (*e.g.*, the carbon cycle in Mohan *et al.*, 2009) – our focus is on findings that trace conceptual development across school years of lower and upper secondary education.

In recent years, a substantial body of literature has been compiled on students' conceptual understanding of chemical reactions. For example, Hadenfeldt *et al.* (2014) systematically reviewed studies on students' understanding of matter, incorporating findings on chemical change. They identified hierarchically structured levels of progression, ranging from a lack of a conceptual model (*e.g.* García Franco and Taber, 2009) to a sophisticated understanding of the processes underlying chemical reactions (*e.g.* Treagust *et al.*, 2010). Some studies have already addressed how these understandings develop over time. For instance, Boo and Watson (2001) traced how scientific explanations of reactions evolve across grade levels within the same group of learners. However, their work was limited to reactions in solution and focused on individual aspects (*e.g.*, bond breaking, collisions, or thermodynamics) rather than their cumulative interplay. Moreover, they did not consider factors that shape students' conceptual development, such as prior knowledge or instructional strategies. More generally, many existing studies concentrate on a single point in schooling (*e.g.* Hesse and Anderson, 1992) or rely on cross-sectional designs (*e.g.* Ahtee and Varjola, 1998). Thus, Hadenfeldt *et al.* (2014) conclude that there is a strong need for studies that examine learning progressions.

The lower secondary level has already been well investigated (Emden *et al.*, 2018; Celik, 2022; Walpuski and Celik, 2024), resulting in empirically validated learning progressions that suggest a gradual development of submicroscopic understanding. However, there is, to the best of our knowledge, rather limited evidence on the upper secondary level. In a comprehensive study on students' understanding of the matter concept, for example, Hadenfeldt *et al.* (2016) also included the concept CR. On the one hand, it was shown that across all school years that were included the understanding of chemical reactions was noticeably lower than that of the other big ideas (structure and composition, physical properties and change, and conservation). On the other hand, due to a lack of suitable learning opportunities and a lack of statistical fit, the items covering higher-level understanding (reorganization of particles and bonds, explaining and justifying reaction processes) had to be removed from the analysis. However, it is precisely the content covered by these items that elicits the difference between learning opportunities at the lower and upper secondary education levels. In the latter, learners should acquire a systematic understanding of chemical reactions as the result of complex interactions of (subatomic) particles, which seems to be a learning hurdle that is difficult to overcome in the context of school learning (Hesse and Anderson, 1992; Ahtee and Varjola, 1998). This gap in research was systematically explored, at least for undergraduate students by Yan and Talanquer (2015). The authors were able to identify overarching conceptual modes from various examples of chemical reactions in an interview study. These conceptual modes concern reasoning processes about the chemical mechanism (how a reaction takes place) as well as chemical causality (why a reaction takes place), and, at a more detailed level, focus on the start, the progress, and the end of a chemical reaction. Conceptually, a more sophisticated understanding represented by these modes is inherently tied to the topics, chemical kinetics and chemical equilibrium (see also Talanquer, 2021), which we understand as relevant "progression factors" and refer to as topic areas in the following. Although Yan and Talanquer (2015) provided important insights into learners' explanatory patterns – both regarding chemical mechanism and chemical causality – the authors' findings remain predominantly qualitative. Moreover, reported results were limited to a relatively small sample that only included students who had already obtained a high school diploma (*i.e.*, undergraduate students and beyond). It was shown that learners at all educational levels in the study tend to use agentive arguments in their explanations of chemical reactions. Encouragingly, however, the cross-sectional data also revealed developmental trends from the early undergraduate level to the advanced graduate level. While learners from the former level were generally unable to provide explanations at the molecular level, at least some learners of the latter level were able to provide mechanistic explanations including multiple interactions between various agents.

Highlighting the research gap. Building on the theoretical considerations outlined above, we note that there are only limited findings on students' individual conceptual development throughout secondary education. With regard to instruction, little is known about conceptual development in connection with targeted teaching within the topic areas of chemical kinetics and chemical equilibrium that we have identified. Although extensive research has addressed these factors, focusing on alternative conceptions (Hackling and Garnett, 1985; Banerjee, 1991; Hesse and Anderson, 1992; Van Driel, 2002; Cakmakci *et al.*, 2006; Özmen, 2008; Cakmakci, 2010) and topic-specific difficulties (Kousathana and Tsaparlis, 2002; Akkus *et al.*, 2003; Justi, 2003; Cakmakci and Aydogdu, 2011; Seçken and Seyhan, 2015; Monteiro *et al.*, 2020), the impact of systematic learning opportunities on students' sophistication in understanding chemical reactions remains widely unexplored. Research by Yan and Talanquer (2015) suggests that moving beyond the submicroscopic understanding typically acquired by the end of lower secondary education is associated with a quantitative understanding of chemical reactions, which is particularly fostered through instruction in the two key topic areas of kinetics and equilibrium.

In the present study, we therefore examine the extent to which instruction on the identified topic areas influences the development of students' reasoning about chemical reactions. As a particular feature of our study, some classes received instruction only on chemical kinetics (kinetics-only group, KOG) while others also received instruction on chemical equilibrium (kinetics-and-equilibrium group, KEG). Importantly, this differentiation was not part of the original design, as we generally recommend that students receive instruction in both topic areas, but it emerged from time-related constraints in some classes. However, this "naturally" occurring variation provided an opportunity to examine the differential contribution of the two topic areas to students' developing understanding of chemical reactions. We assume differences as prior research suggests that instruction on chemical equilibrium introduces additional conceptual resources, particularly related to energetic considerations and the dynamic nature of chemical systems. Moreover, these ideas may support students in developing a more differentiated understanding of reaction systems and in distinguishing different reaction systems.

In doing so, we contribute to the existing body of research by providing insights into time-related conceptual learning within the same group of learners after several weeks of instruction (see Methods). The study therefore evaluates changes in conceptual understanding following a research-informed TLS. While the empirical evidence generated at this stage of the study is not yet sufficient to claim an empirically validated learning progression, our findings can inform the design and the subsequent empirical investigation of a learning progression. In this way, our findings may help move towards a validated LP for upper secondary education, similar to those that are already existing for lower secondary education.

Shaping conceptual development

In addition to instructional opportunities, further cognitive and affective factors shape individual conceptual development. **Prior knowledge** in the context of chemical reactions may shape how learners interpret and benefit from subsequent learning opportunities (Etzel *et al.*, 2025), as more advanced concepts often build on earlier forms of understanding (cumulative conceptual understanding). For instance, understanding the relationship between activation energy and the Maxwell–Boltzmann distribution presupposes an understanding of particle collisions and interactions. If these earlier ideas are not sufficiently integrated, learners may struggle to connect more advanced concepts and revert to simpler reasoning patterns. This aligns with the notion that prior knowledge is particularly influential when it is congruent with new learning content (Brod, 2021; Edelsbrunner *et al.*, 2024). We therefore distinguish between two perspectives on prior knowledge: (1) general prior knowledge, reflected in students' previous chemistry grade and (2) specific and congruent prior knowledge, reflected in learners' conceptual modes prior to instruction. Because conceptual modes build on one another while increasing in explanatory power, they can be understood as cumulative, suggesting that learners' understanding at the end of lower secondary education strongly shapes subsequent learning. This also highlights the importance of closely diagnosing students' explanatory patterns, particularly during transitions between school levels.

In addition, subject-related interest may shape conceptual development, particularly in less familiar contexts where transfer cannot be assumed (Schwartz *et al.*, 2005). Subject-related interest has been associated with increased cognitive engagement and academic performance (Marsh *et al.*, 2005; Hidi and Renninger, 2006). While the focus of the present studies is on cognitive learning gains in students, we included subject-related interest as an exploratory covariate to isolate instructional and prior knowledge effects from potential interest-related influences.

Research questions and hypotheses

Based on the theoretical considerations regarding conceptual development and targeted instruction, the following research questions were derived:

Research question 1

To what extent do upper secondary students' conceptual modes regarding the mechanistic interpretation of chemical reactions change after working in a learning environment on chemical kinetics (and chemical equilibrium)?

Given the strong relationship between the content-related description of conceptual modes and the content taught in the context of a research-informed TLS covering these topic areas (Yan and Talanquer, 2015), we expect an observable shift in students' conceptual modes of chemical mechanism towards a higher explanatory power. However, we also expect to descriptively observe that the shift to conceptual modes with higher explanatory power is favored when learners start from a certain baseline level of understanding (Edelsbrunner *et al.*, 2024).

Research question 2

To what extent does this change differ for students who only received instruction on chemical kinetics (kinetic only group, KOG) and those who received instruction on both topic areas (kinetic and equilibrium group, KEG), also depending on the specific reaction example used?

As Yan and Talanquer (2015) showed, students' expressed conceptual modes are highly dependent on the chosen reaction example. We therefore also assume to observe these differences when comparing two different reaction types (complete combustion reaction and incomplete esterification) that we chose for our investigation (further details are provided in the 'instruments' section). In the case of these two reaction types, it is plausible that some learners will incorrectly assume the establishment of a dynamic equilibrium even in the case of a complete reaction. Such overgeneralized application of a newly learned concept is known as negative transfer (Woltz *et al.*, 2000). This risk may be particularly relevant for learners in the KEG condition, as they were explicitly taught about dynamic equilibrium. However, the instructional unit explicitly categorized and contrasted different reaction systems in order to support learners in differentiating between complete reactions and equilibrium reactions. Such categorization processes can promote deeper concept formation (Goldwater *et al.*, 2018). Therefore, despite the possibility of negative transfer, we do not expect substantial overgeneralization in the KEG group when interpreting the end of complete reactions. In addition, we expect moderate advantages in explaining the start and progress of reactions for students who have been taught both topic-related subsets (KEG), as these students had more learning opportunities to deal with chemical reactions in general, which, for example, can be interpreted as time on task (*e.g.* Hattie, 2010).

In turn, we do expect substantial differences between KOG and KEG regarding the interpretation of incomplete reactions. As the evaluation of systemic conditions leading to the establishment of a dynamic equilibrium, reflecting the conceptual organization from complete to incomplete chemical reactions (Van Driel *et al.*, 1998), is only taught in KEG, we assume that there will be overall a greater shift to conceptual modes with a higher explanatory power in this group.

Research question 3

What influence do prior conceptual modes and students' last chemistry grade have on the outcome modes when accounting for subject-related interest as an exploratory covariate?

As previously discussed, we assume students' prior conceptual modes to be strong predictors of their outcome modes because their order in explanatory power can be understood as a cumulative progression, and they represent highly specific prior knowledge. This type of prior knowledge is relevant and strongly related to the new knowledge components to be acquired and should therefore have a significant positive effect on the conceptual development (Brod, 2021; Edelsbrunner *et al.*, 2024). In addition, we also assume students' grades to have a slight to moderate positive effect on the outcome modes, since this can also be seen as a proxy for general prior knowledge. However, we hypothesize that this effect will be smaller than the effect of students' prior conceptual mode, as the participants' grade is much more general and, in this sense, less relevant and related to the new concepts. Subject-related interest may also show a positive association with students' outcome modes and was therefore considered to control for potential confounding effects.

Methods

Ethical considerations

Informed consent was obtained from all participants. Participation was voluntary, and confidentiality and anonymity were ensured. The study was conducted in accordance with institutional ethical standards and approved by our local ethical committee (ID 2022_33_KU).

Sample

Sample description. The sample included 14 classes from German schools, comprising 9 classes from *Gymnasien* (academic-track secondary schools) and 5 classes from comprehensive schools. The classes were drawn from two federal states: 13 classes from Schleswig–Holstein and 1 class from Rhineland–Palatinate, thus a strong representation of northern German schools. These classes were taught by 13 different teachers, with one teacher responsible for teaching two different classes. The surveys took place during the 2022/2023 school year and covered a period from September 2022 (first pre-test) to July 2023 (last post-test). In total, the participating classes included 245 students. However, 183 students (55.1% female, 43.3% male, and 1.6% non-binary) could be included in the analysis, as these were students who were present at both pre- and post-measurements. Participation was voluntary, and both school administration and students (or their legal guardians) provided informed consent for participation in the study. German was by far the most spoken language, accounting for 87.8% of the participants. This was followed by 1.1% Arabic, 1.1% Turkish, 9.5% other languages and 0.5% uncertain (*e.g.* participants who did not clearly specify their most spoken language). The average last chemistry grade of the sample was 2.52, which, according to the German grading system, falls between "good" (2) and "satisfactory" (3). However, the full range of grades, from "very good" (1) to "insufficient" (6), was represented within the sample. Teachers were able to decide whether to participate in the study based on the topic, and due to typically non-fixed thematic sequences within upper secondary education, the grade levels (11th grade to 13th grade) varied. However, grade 11 was most frequently represented, which marks the beginning of upper secondary education in the federal states. Thus, the age range, which we did not explicitly collect, typically falls between 16 and 18 years.

Participants' expected prior knowledge. Since all participants had completed the transition to the upper secondary level, we synthesized the learning-relevant competence goals that should be met by the end of lower secondary education on the basis of regional curricula from the two federal states (Ministerium für Bildung, Wissenschaft, Jugend und Kultur, 2010; Ministerium für Bildung, Wissenschaft, Weiterbildung und Kultur, 2014; Ministerium für Bildung, Wissenschaft und Kultur des Landes Schleswig–Holstein, 2019). A detailed summary of these goals can be found in the appendix (Section A and Table A1). Given that many of the participating students received much of their prior chemistry instruction during the COVID-19 pandemic, it is reasonable to infer that certain content-specific learning objectives may not have been fully achieved (Betthäuser *et al.*, 2023; Lewalter *et al.*, 2023).

Overall, both curricula introduce chemical reactions at the submicroscopic level primarily through the breaking and forming of chemical bonds. Although activation energy is included, it is usually presented superficially as an energy barrier that must be overcome, reinforcing the idea of heat as an external trigger rather than relating it to molecular energy distributions (Pölloth *et al.*, 2023). Prior research suggests that this qualitative treatment limits students' understanding of why increasing temperature leads to more successful collisions (Justi, 2003). Despite minor differences in phrasing and exemplarity, both curricula target a similar competence level by the end of lower secondary education: students should explain reactions using the particle model, describe energy changes, and understand bond breaking and formation. Deeper mechanistic insights are reserved for upper secondary education, where kinetic and equilibrium principles are addressed more systematically. Although Rhineland–Palatinate briefly introduces first equilibrium concepts through reversibility, the dynamic establishment of equilibrium is not treated, leaving mechanistic understanding largely underdeveloped.

Study design. We conducted the study as a pre–post design over an extended instructional period. During this period, students participated in a digitally supported, TLS-oriented teaching unit, which is described below together with the assessment opportunities forming the basis of the investigation.

Teaching unit. The learning opportunities for the two topic areas are part of a comprehensive teaching unit that lasts several weeks (approx. 10 weeks at 2 lessons per week) and has been implemented as a digital learning environment in the learning management system (LMS) Moodle (for a structure and content overview see Table 1). In relation to the overarching goal of the project, the implementation of the digital variant was chosen to develop learning environments based on the framework by Kubsch *et al.* (2022). This framework provides a structured approach for integrating meaningful, inquiry-oriented learning opportunities in the sense of project-based learning and is guided by epistemic activities embedded in digital learning environments. The – in most cases novel – LMS-supported unit was piloted in spring and summer 2022 to identify implementation and comprehension challenges. Based on weekly exchanges with the participating teacher, the unit was revised and key elements for teacher PD were derived. For the main study, all teachers attended a PD session and received a detailed teaching guide with lesson plans to support implementation fidelity. Nevertheless, teacher-specific

Table 1 Structure of the digital learning environment in lesson sets with accompanying pre- and post-test and the corresponding content covered in each lesson set

Lesson set	Progression step	Content	Contexts
Pre-test (approx. 90 minutes)			
Introduction to using Moodle (for learners)			
1	Quantitative dynamics of chemical reactions	• Definition of the concept of reaction rate • Appropriate metrics for measuring reaction rate • Distinction between the average and instantaneous reaction rate	• Wheat flour reacts at different speeds (digesting a bread roll, rising yeast dough, flour dust explosion)
2	Control and prediction of chemical reactions	• Modelling the reaction processes using the collision model • Prediction and explanation of various factors influencing the course of reaction • Catalysis and alternative reaction pathways	• Influence of acid concentration and temperature on the dissolution of fizzy dietary supplement tablets • Food spoilage and metabolism
3	Dynamic equilibrium	• Reaction incompleteness and its causes • Systemic conditions for equilibrium adjustment • Characterization of the equilibrium state	• Production process of banana flavor
4		• Manipulation of the equilibrium state	• Industrial applications using the example of nitrogen fertilizers
Post-test (approx. 60 minutes)			

variations over the more than ten-week implementation period cannot be fully controlled.

As mentioned earlier, KOG completed lesson sets 1–2, while KEG completed all lesson sets. The four lesson sets for this unit were systematically built on the three steps of analyzing quantitative dynamics of chemical reactions, predicting and controlling chemical reactions, and analyzing dynamic equilibria to enable cumulative learning within the core concept of chemical reactions. In the instructional design, we also included reviews of conceptual difficulties (Bain and Towns, 2016; Heeg *et al.*, 2020) and considered basic multimedia instructional strategies (Mayer, 2021) as well as specific digital tools (*e.g.* Lossjew and Bernholt, 2024). Table 1 shows that the content of lesson sets 2–4 was strongly informed by the empirical findings of Yan and Talanquer (2015) on how students interpret the start, progress and end of reactions mechanistically. In line with the increasing explanatory power of conceptual modes, we successively incorporated these elements into the instructional design, which therefore forms an empirically grounded TLS. Table 1 further illustrates that we embedded the domain-specific content in interrelated sub-contexts to provide relevance to the otherwise rather abstract content (Parchmann *et al.*, 2006; Schneider *et al.*, 2020). In summary, the unit aimed to shift students' understanding of chemical reactions from a descriptive to a predictive, process-oriented view through cumulative learning opportunities. The instructional unit can be provided by the authors as a Moodle course upon request. Translation into English or any other language other than German would be required.

Available data. The pre- and post-tests were administered *via* the Moodle test tool. While the digital implementation allowed us to capture all learner artifacts across ten weeks, this article focuses on the pre- and post-surveys to examine conceptual development within the core concept CR following instruction in upper secondary education.

Instruments

Assessing conceptual modes. To assess learners' conceptual modes in the pre- and post-tests, we developed five open-ended questions based on the qualitative description of different conceptual modes by Yan and Talanquer (2015) for two reaction examples (Table 2). As part of the piloting phase (see the Teaching Unit section), we examined the questions regarding (1) content validity, specifically whether learners addressed the intended conceptual aspects, and (2) comprehensibility. We could confirm both aspects based on the piloting results. In addition, the content validity of the items was discussed with colleagues with expertise in chemistry education. From a content perspective, we have selected a combustion reaction and an esterification reaction to cover both complete and incomplete reactions that learners are not completely unfamiliar with, based on the previous curriculum. From an assessment perspective, we developed the questions to address the start of the reaction (2 questions for each reaction type), the further course or progress of the reaction (1 question each) and the end of the reaction (2 questions each), thus corresponding to the three-part classification of conceptual modes for chemical mechanism by Yan and Talanquer (2015). Based on the literature synthesis and the proposed TLS, we focused on the chemical mechanism, as no substantial progression in chemical causality was expected within the scope of our instructional unit. Fig. 1 shows the development of an instrument for quantitatively assessing students' conceptual modes regarding the start, progress and end of a reaction, based on an extension to the work of Yan and Talanquer (2015).

As shown in Fig. 1, testing the developed scoring guides led to a refinement process. For this purpose, a substantial proportion (approximately 30%) of the free-text responses were evaluated by human raters, followed by a discussion of issues related to the differentiation of response quality. It was noted that some learners incorporated the concept of particle collisions, but in a relatively generic and undifferentiated manner. In contrast, other responses described collisions as a necessary prerequisite for further processes (*e.g.* bond breaking and reformation). To address this qualitative content difference, we refined the scoring guide by dividing "random collisions" and "changes through interactions" into "simple collisions" and "advanced collisions". This refinement process results in an adapted version of conceptual modes on chemical mechanism (see Fig. 2) that is based on the analysis of all written student responses (Fig. 1).

While two independent coders had already been involved in this refinement process as part of their training, the entire dataset was subsequently coded using the final scoring guide. Importantly, this guide did not solely rely on specific keywords but focused on the conceptual meaning of students' responses, including examples and boundary cases to account for variability in students' writing and expression. Based on sub-mode descriptions and authentic examples (see Table 2), each response was assigned to a corresponding sub-mode. Approximately 20% of the dataset was coded by both coders, and interrater reliability was calculated on this basis (see Table 2), yielding satisfactory results across all main modes. Table 2 illustrates the open-ended questions addressing the three levels of conceptual modes using the example of the combustion reaction. The detailed sub-modes are also presented, along with sub-mode descriptions and respective student examples. An analogous table for the esterification reaction is provided in the supplementary information (SI).

Subject-related interest. To measure subject-related interest, we used a common scale for German-speaking countries, consisting of 4 items rated on a 4-point Likert scale ranging from "does not apply at all" and "fully applies" (Daniels, 2008). The scale demonstrated good internal consistency with an overall Cronbach's α of 0.84. The item specific values ranged between 0.78 and 0.85. Example items include "I find chemistry exiting" or "I am eager to learn more about chemistry". The analysis of internal consistency was conducted using the *psych* package in R (version 4.4.1).

Other background variables. In addition to the aforementioned variables, we assessed further background variables (most commonly spoken language, grade and gender), of which the last chemistry grade is used in this study as a proxy for general prior knowledge. Grades were coded with the German

Table 2 Overview of modes and sub-modes with increasing explanatory power. In addition, a description, an example and the inter-rater reliability per mode are given

Mode	Open text item[a]	Sub-modes	Description	Student example	Cohens κ
Start (MS)	(1) Describe what happens to the carbon and oxygen particles when they are heated, *i.e.* before the actual reaction begins, so that a reaction can occur	Advanced collision (COLEXP)	Students use the concept of random effective collisions and resulting (electronic) interactions to explain the reaction start	Oxygen molecules move at a certain speed and collide with the vibrating carbon atoms. Once the particles randomly collide with sufficient kinetic energy (which is increased by the Bunsen), the reaction begins	0.71 (pre); 0.81 (post)
		Simple collision (COLSIMP)	Students use the concept of random collisions without further interactions	As soon as two molecules collide, a reaction occurs	
	(2) Explain why heating the mixture causes the reaction to start immediately and why the reaction does not stop immediately when the Bunsen is removed	Mutual attractions (ATTRAC)	Students use the concept of mutual attraction to explain the start of reaction	Attractive forces between oxygen molecules and carbon atoms cause the two particles to approach each other, initiating the reaction	
		Initial factor[b] (INIT)	Students use the concept of an initiating substance (reactivity) or name external factor as reason for the reaction start	The heat from the burner breaks bonds in oxygen molecules, allowing them to react with carbon atoms	
		No concept (NOCONC)	No concepts are used to explain the reaction start	CO_2 is formed in this reaction	
Progress (MP)	(3) Describe how you imagine the reaction at the particle level to proceed	Advanced collision (COLEXP)	Students use a combination of different interactions (continued collisions – including product particles, bond breaking/forming, escape/remaining of a substance in the system) to explain the progress	Oxygen molecules and carbon atoms continue to collide and can rebound from each other. However, if the kinetic energy is sufficient, the collisions will lead to further reactions. Since the reaction of the particles themselves releases energy, the reaction continues and newly formed CO_2-molecules leave the open system	0.81 (pre); 0.85 (post)
		Simple collision (COLSIMP)	Students use the concept of perpetual collisions without describing further interactions	The molecules continue to collide and thus react. They can also rebound after colliding	
		Bond breaking and reformation (BONDS)	Students only use the concept of bond breaking/forming to explain the progress	New bonds between carbon-atoms and oxygen-atoms are formed and old ones are continually broken	
		Macroscopic change of substances (MACRO)	Students describe the course of the reaction from a substance-based perspective (*e.g.* increase in products/decrease in reactants	More and more carbon and oxygen react with each other, so that more and more carbon dioxide is formed	
		No concept (NOCONC)	No concepts are used to explain the progress	The round flask is getting warm	
End (ME)	(4) Describe how you imagine the end of the reaction at the particle level. Which particles are still present at this point?	Dynamic equilibrium (DYNAMIC)	Students explain that reactions do not actually end, but instead reach a state of dynamic equilibrium	Although the ratio of carbon, oxygen and carbon dioxide no longer changes, reactions continue to take place at the particle level, in both directions at the same speed	0.85 (pre); 0.91 (post)
		Static equilibrium (STATIC)	Students explain the end of the reaction by the achievement of a static equilibrium	At some point, the ratio of carbon, oxygen and carbon dioxide no longer changes; at this point, equilibrium has been reached and no more reactions take place	
	(5) Explain why the reaction potentially stops at this point at what factors influence the end of the reaction	Limiting component (LIMIT)	Students explain the reaction end by the presence of a limiting factor and/or by a complete reaction of the reactants	Carbon is the limiting factor, as oxygen is present in excess. The reaction stops when the limiting factor is used up	
		No concept (NO-CONC)	No concepts are used to explain the reaction end	At some point, the flask is empty	

[a] Questions were translated from German. [b] As initial factors, we included both the mention of single compounds as an initiator and external factors.

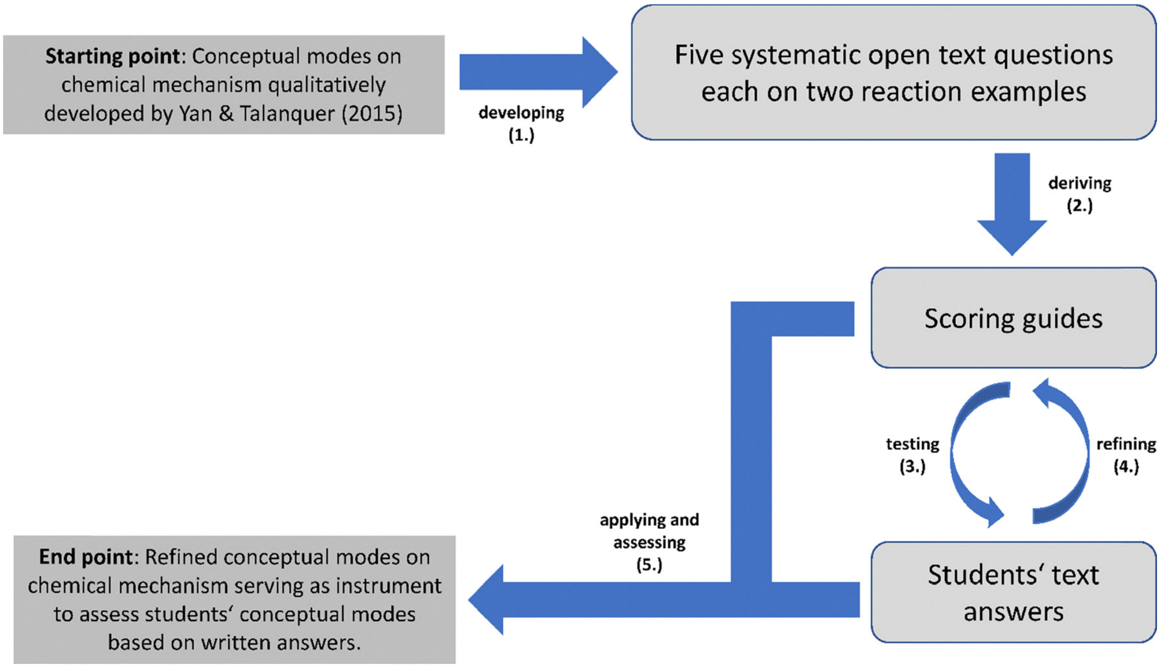

Fig. 1 Process steps for designing and implementing a quantitative instrument to capture the conceptual modes on the chemical mechanism of learners in upper secondary education.

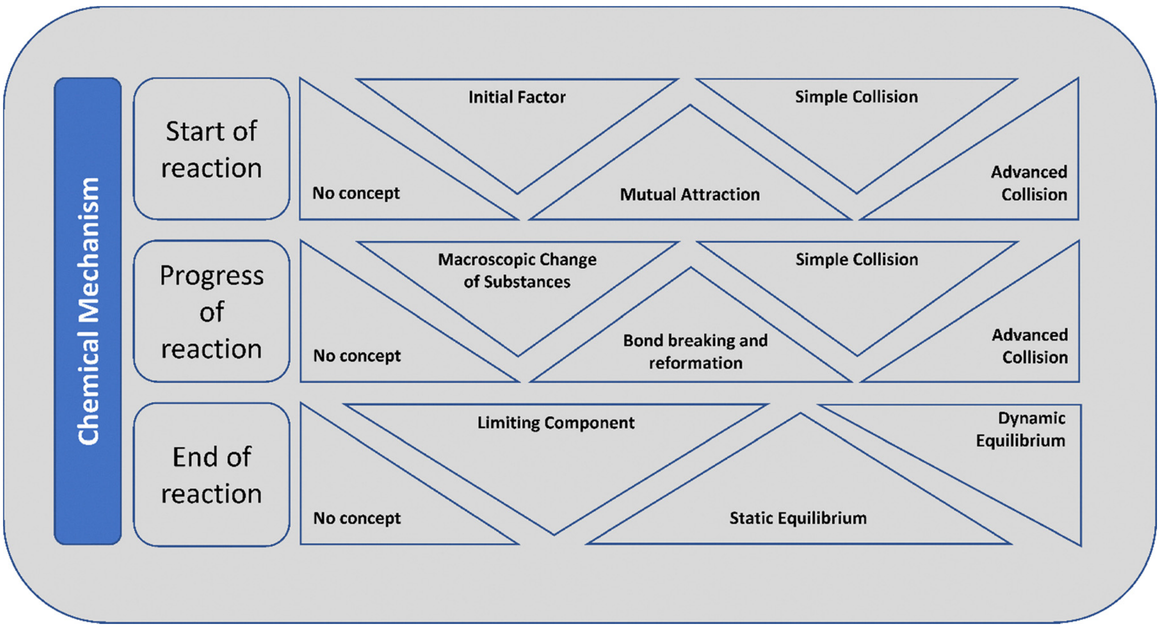

Fig. 2 Refined conceptual modes on chemical mechanism, adapted from Yan and Talanquer (2015).

1–6 grading scale, with 1 representing the best grade and 6 the worst.

Data analysis

The analyses are informed by the qualitative findings on cross-sectional development in the core concept CR by Yan and Talanquer (2015) and apply inductively derived conceptual modes in a comprehensive sample of learners before and after having received instruction on the progress-related topics, chemical kinetics and chemical equilibrium. The authors elaborated the conceptual modes' connectedness with the specific reaction example. This leads, in addition to the clear differentiation between modes (start, progress and end of the reaction), to the fact that we also did not cumulate the modes expressed by learners into an aggregated overarching ability, but have rather considered differential changes per mode and per reaction example (3 × 2 schemes).

Analytical steps. To address the different research questions, we employ diverse methods that align with the specific epistemological focus of each question. Fig. 3 serves as an advance organizer for the methodological triad which we will explicate in the following.

First, regarding RQ1, we aim to analyze overall changes in the distribution of participants across the different conceptual sub-modes (*cf.* Table 2) before and after the teaching unit. For this purpose, we first observed shifts in students' conceptual sub-modes directly from the contingency tables. These observable shifts were identified as changes in the frequency of students in (especially higher) sub-modes as well as by the transitions between sub-modes from before to after the teaching unit. To further analyze these shifts, we calculated a test of marginal homogeneity (also known as the Stuart–Maxwell test), which can be applied to paired samples to assess whether changes in the marginal distributions of squared contingency tables are statistically significant (Stuart, 1955). This analysis was performed using the package *DescTools* in R (version 4.4.1).

Second, as described in our research gap, some of the participating classes received instruction only on chemical kinetics (KOG), while another subset of students was additionally taught chemical equilibrium (KEG). This difference in instructional content effectively creates a treatment group (KEG) and a corresponding comparison group (KOG). To assess the effect of this additional instruction (RQ2), we analyze how the transitions between conceptual modes differ between these groups over time. Specifically, we compare the change in conceptual mode occupancies before and after instruction within each group; these represent differences in the conceptual modes over time. We then analyze how the magnitude of these changes differs between the two groups, *i.e.* group-related differences due to differential instruction. This approach, known as Difference-in-Differences (DiD, Graves *et al.*, 2022), is also visualized in Fig. 3 to better capture its idea. It allows us to isolate the effect of the additional instruction by accounting for general learning trends in both groups. More specifically, we employed the extended additive DiD approach for categorial outcomes (Graves *et al.*, 2022). To quantify group-related differences, an Average Effect of Treatment on the Treated (ATT) is calculated for all occupancy levels. The ATT estimates the causal effect of an intervention (in this case additional learning opportunities on chemical equilibrium) for those individuals who actually received the treatment – that is, the extent to which their probability of occupying a certain post-sub-mode is higher or lower compared to what would be expected without intervention. Further details for our choice of the additive approach and a detailed description of the ATT estimation procedure can be found in the appendix (Section C). This analysis was performed using the packages *fastDummies* and *ggaluvial* in R (version 4.4.1).

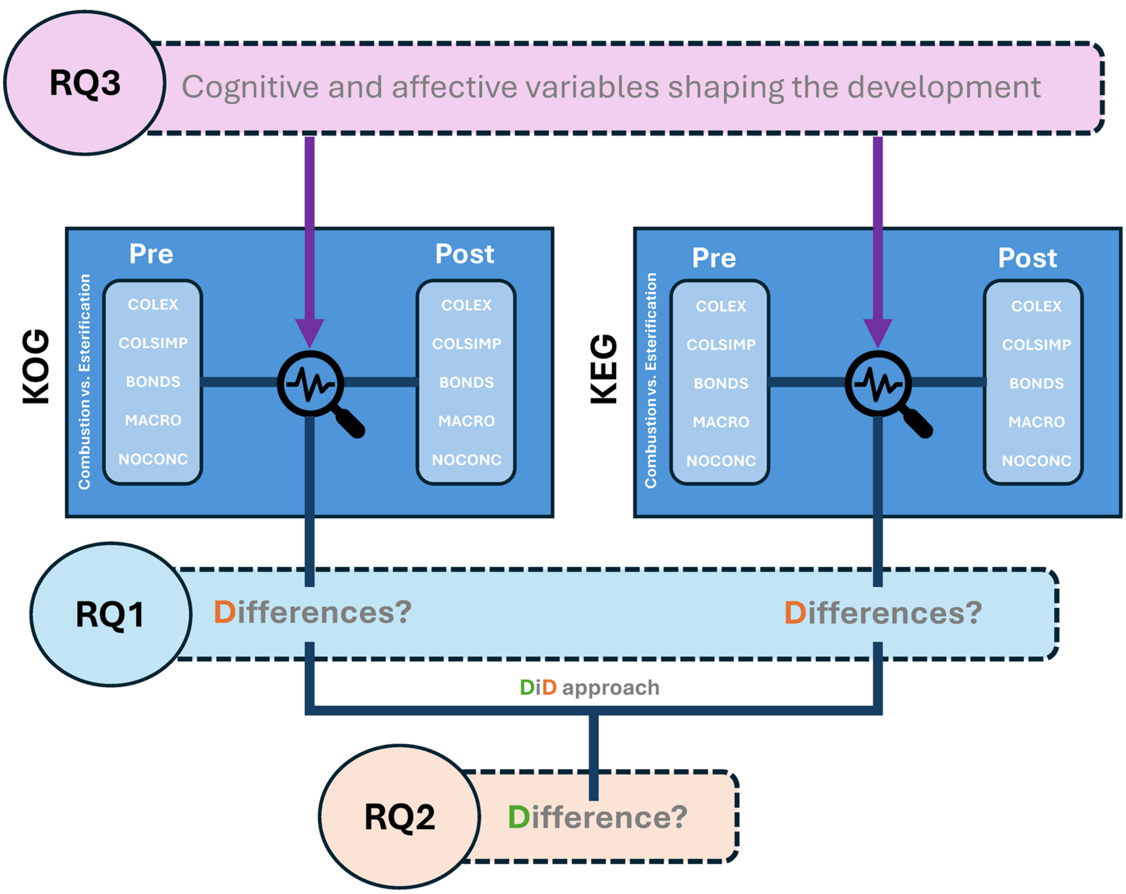

Fig. 3 Overview of analytical steps linking their specific focus to the outcome measures.

Third, we analyzed how different predictors influence the likelihood of being in a higher conceptual mode after the teaching unit (RQ3). While the Stuart–Maxwell test (see RQ1) can determine whether the marginal distributions before and after the teaching unit differ significantly, it does not allow for conclusions about the dependencies between pre- and post-sub-modes. However, these dependencies reflect the influence of specific prior knowledge (Edelsbrunner *et al.*, 2024) and, thus, the potential for taking advantage of new learning opportunities (Etzel *et al.*, 2025). Accordingly, the analysis aims to provide insights into the cumulative structure of conceptual modes. Moreover, additional control variables (chemistry grade, interest) were included to allow for the isolation of the effects of specific prior knowledge. To integrate these considerations analytically, we conducted an ordinal regression analysis (Hosmer and Lemeshow, 2000) as a final modeling step. Ordinal logistic regression is a method used to analyze the influence of various predictors on an ordinal dependent variable – one that has a natural ranking but unknown intervals between categories. Treating conceptual modes as an ordinal outcome variable is based on the theoretical assumption that higher modes exhibit increasing explanatory power, making ordinal logistic regression the appropriate method to analyze how different predictors influence the likelihood of being in a higher mode. We developed the regression models incrementally using a manual forward stepwise logistic regression approach that was guided by theoretical considerations (see appendix for details on the model-building process). In these regression models, the pre-sub-modes (specific prior knowledge) were consistently treated as ordinal predictors. Consequently, we computed two model variants: (a) using NOCONC as the reference category to assess the predictive power of higher pre-sub-modes compared to the absence of concept activation in the pre-condition, and (b) introducing contrast coding to examine the predictive strength of each pre-sub-mode relative to the next lower category. This dual strategy allowed us to capture both the distinction from NOCONC and the incremental effects across the ordinal levels of the pre-sub-modes, thereby offering insight into their cumulative structure. In cases where the effect of a particular pre-sub-mode appeared very large, we investigated whether this was due to extremely low frequencies in the dataset. In all such instances, the respective sub-mode had very few occurrences in the pre-condition, resulting in rather inflated coefficient estimates. This issue results from the low occurrence of certain conceptual sub-modes at the pre-test. Given the learners' expected prior knowledge, it is plausible that only a small number of students will have conceptually advanced modes of reasoning when they enter the instructional unit. To preserve both interpretability and robustness, we excluded such categories from the model and did not report the associated effect. However, this necessary data-driven exclusion imposes limitations on the analysis of the cumulative structure of conceptual modes. We performed several classical checks to ensure the statistical validity of our regression models, which are typical for ordinal regression (*e.g.* multicollinearity or checking for the proportional odds assumption). A more detailed discussion of these aspects can be found in the appendix (Section C). Only the models that met all these criteria were retained. We controlled for instructional groups (KOG and KEG) in every final model. Since the three conceptual modes (start, progress and end of a reaction) were analyzed separately and could differ depending on the reaction example (combustion or esterification), we did not aggregate across modes or reaction examples, resulting in six separate regression analyses. All (pre-)analyses were performed using the packages *car*, *MASS*, *brant* and *Ordinal* in R (version 4.4.1).

Results

We organized this section according to the three analytical steps derived from our three research questions (Part I to Part III). Table 3 summarizes students' grades and subject-related interests across the sample. Of the total sample (N = 183), who participated in both the pre- and post-tests, only 150 students provided responses for these background variables. As a result, the sample size for RQ3 is also reduced to N = 150. As mentioned before, grade was reported on a German grading scale, where 1 represents the highest score and 6 the lowest score. A comparison of these descriptive parameters of both variables in the full sample and the reduced sample is provided in the appendix (Section D) to rule out any bias caused by overachieving or overly interested learners.

Part I: overall changes in students' conceptual modes

Fig. 4 shows for all main modes (start, progress and end) and for both reaction types (combustion, esterification) the pre–post distribution of the respective sub-modes, which directly corresponds to the marginal distributions (*i.e.*, the percentage distributions) at both measurement points. Detailed transition matrices in the appendix complement these results. Overall, the increasing color intensity across all main modes and reaction examples indicates a shift toward sub-modes with higher explanatory power. While Fig. 4 displays changes in the marginal distributions (corresponding to overall changes) before and after the instructional opportunities, we also visualized the transitions between sub-modes for each main mode in Fig. 5–7. These transitions are described in more detail below.

Reaction start. In the pre-condition, many learners do not activate specific concepts when describing the start of a reaction (red part of Fig. 4). Consistent with expectations based on prior knowledge (see expected prior knowledge), the idea of an initial factor (INIT) is most likely taken up in both reactions, while collision theory is largely absent. A key difference is that mutual attractions (ATTRAC) are not activated in combustion reactions but appear in esterification. Overall, esterification seems more conceptually demanding, aligning with curricular

Table 3 Descriptive summary of the predictors, last chemistry grades and subject-related interests

Variable	Total (N)	Mean	SD	Min	Max
Grade	150	2.52	1.15	1.00	6.00
Subject-related interest	150	2.55	0.75	1.00	4.00

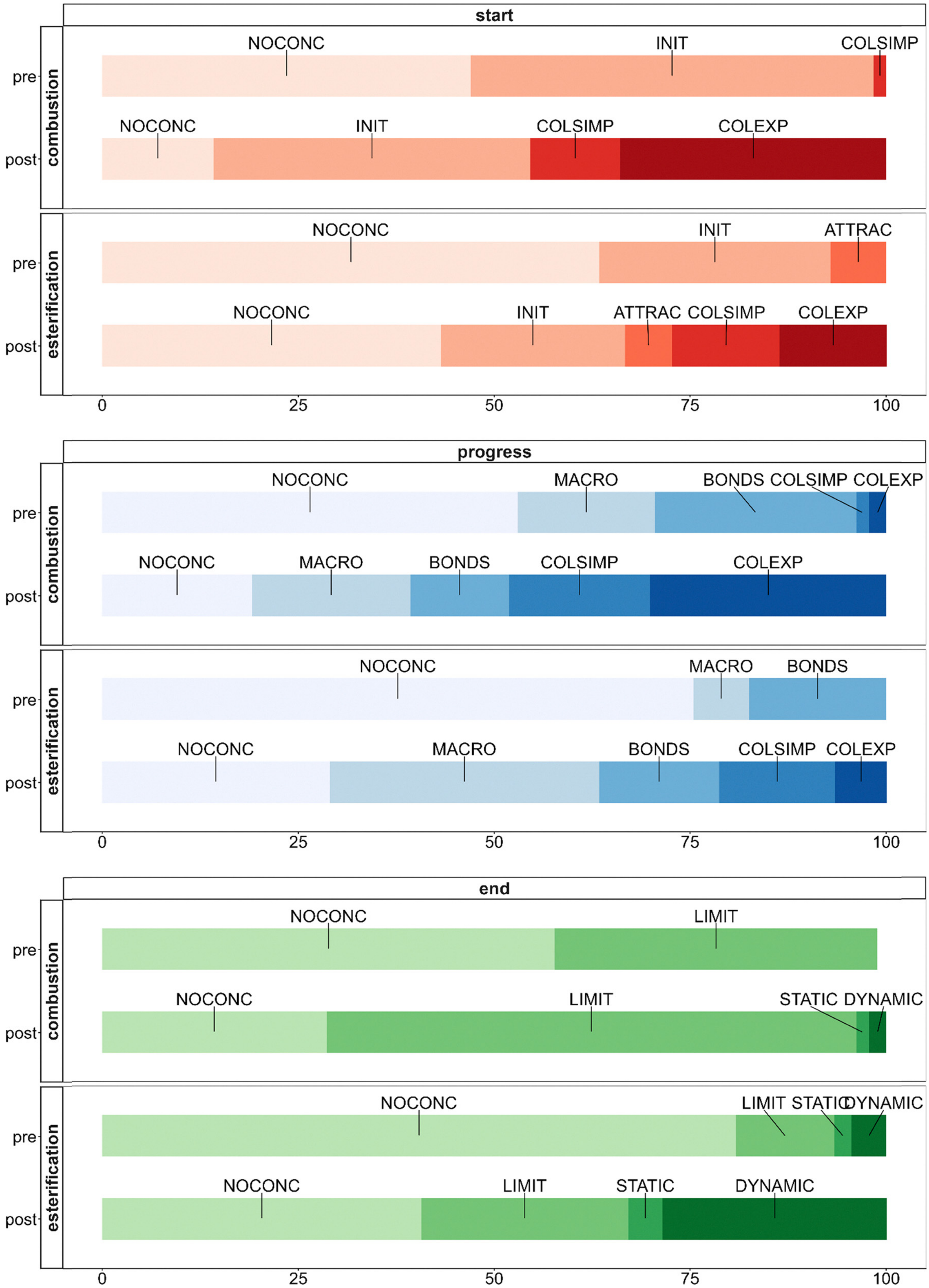

Fig. 4 Pre–post distribution of sub-modes, structured by main mode (*x*-axis) and reaction example (*y*-axis) for the start (red), progress (blue) and end (green) of both reaction types.

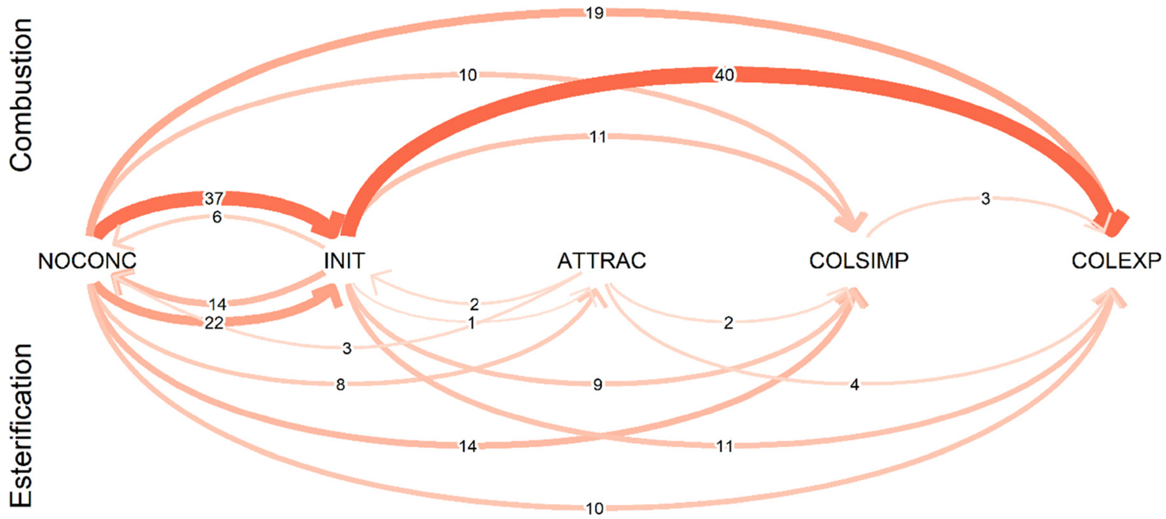

Fig. 5 Transitions between sub-modes from pre to post for the reaction start (upper part: combustion, lower part: esterification). Arrowheads indicate whether transitions are progressive or regressive.

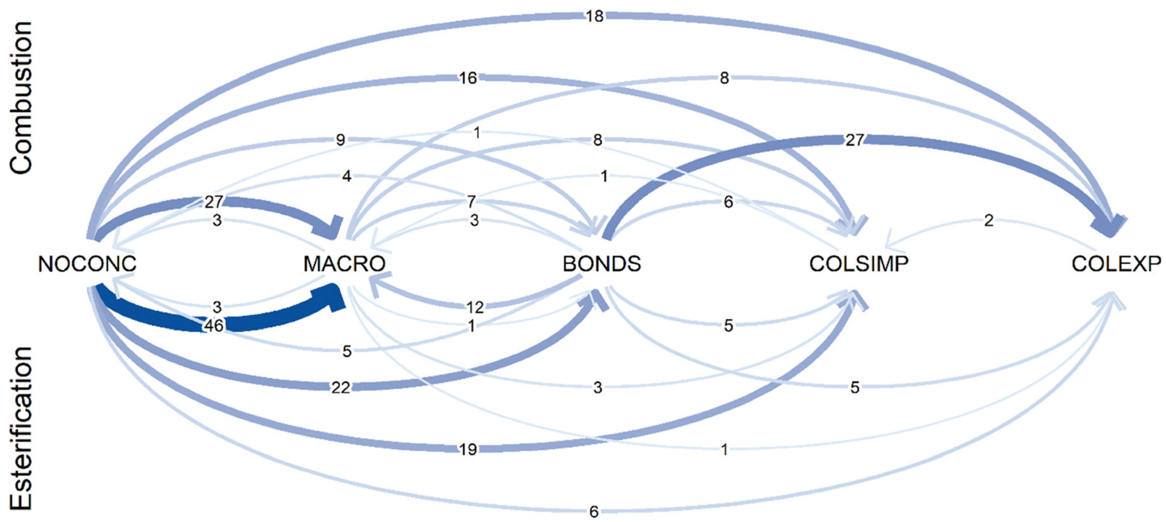

Fig. 6 Transitions between sub-modes from pre to post for the reaction progress (upper part: combustion, lower part: esterification). Arrowheads indicate whether transitions are progressive or regressive.

analyses that emphasize combustion reactions in lower secondary chemistry. This trend is also reflected in the sub-mode transitions from pre to post (see Fig. 5). Although we can observe positive shifts for esterification overall, they are noticeably smaller compared to combustion. At the same time, Fig. 5 shows that the presence of specific prior knowledge favors transitions into higher sub-modes – for example the number of transitions from INIT to a comprehensive understanding of collisions (COLEXP) compared to no concept (NOCONC) to COLEXP. However, this observation requires confirmation (see part III). Regressive transitions occur, but they are overall much less frequent.

Reaction progress. A similar trend is evident for reaction progress (blue part of Fig. 4). Many learners do not activate specific conceptual knowledge in the pre-condition, chemical bonding (BONDS) is the most salient concept. Additionally, a macroscopic focus (MACRO) also seems to take a prominent role. It reflects a primarily correct description of the reaction progress while neglecting submicroscopic considerations – thereby limiting a deeper understanding of energy changes. Although positive conceptual shifts are evident from pre to post, the macroscopic focus (MACRO) remains prominent even after instructional opportunities particularly in the context of the esterification. Fig. 6 shows that in combustion, understanding bond breaking and formation (BONDS) particularly favors transitions to a comprehensive understanding of collisions (COLEXP). In esterification, many learners rely on a macroscopic focus (MACRO) as an explanatory pattern, especially if they had no to little prior concepts (NOCONC). Still, in esterification more learners move from NOCONC to BONDS than from NOCONC to COLEXP, suggesting that this level must be passed cumulatively despite new learning opportunities addressing collision theory.

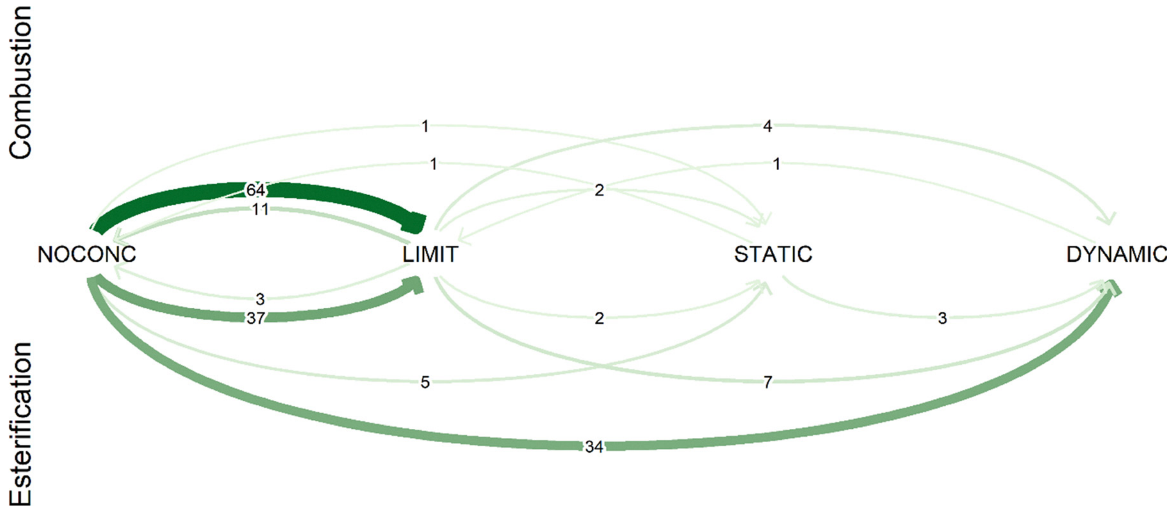

Fig. 7 Transitions between sub-modes from pre to post for the reaction end (upper part: combustion, lower part: esterification). Arrowheads indicate whether transitions are progressive or regressive.

Reaction end. In the pre-condition, specific concepts are rarely activated when interpreting the end of a reaction (green part in Fig. 4). This is not unexpected, as lower secondary chemistry usually treats reactions as going to completion (Van Driel, 2002). The limiting factor (LIMIT) emerges as the most salient sub-mode. In the post-condition, clear shifts appear, with combustion remaining correctly dominated by the limiting factor, while esterification shows a more balanced distribution among no concepts (NOCONC), the limiting factor (LIMIT) and a dynamic understanding of equilibrium (DYNAMIC). For esterification, a static understanding (STATIC) is largely irrelevant as both a starting and endpoint. In contrast, LIMIT and DYNAMIC show different patterns: in combustion, transitions to LIMIT dominate, whereas transitions from NOCONC are roughly balanced between LIMIT and DYNAMIC in esterification.

Significance of changes in the marginal distributions. Overall, the tests of marginal homogeneity suggest that the marginal distributions changed substantially across both reaction examples and the total of their specific conceptual modes, thus indicating conceptual learning through instruction. However, these descriptive insights and the test of marginal homogeneity do not allow for cell-level inferences about how learners' pre-instructional sub-modes shape subsequent development (see Part III). Detailed test results for all comparisons can be found in the appendix (Table A7).

Part II: differential changes in students' conceptual modes

We examined differences between the instructional groups (KOG and KEG) using an additive DiD approach, resulting in ATT estimators. The ATT estimator quantifies the average causal effect of receiving instruction on both kinetics and equilibrium (KEG) compared to kinetics only (KOG). For conceptual sub-mode occupancy (0–100%), a positive ATT indicates a higher probability of occupying a sub-mode in KEG, while a negative ATT indicates the opposite. In our report, the ATT consistently refers to the KEG group. For example, an ATT of 0.094 for the start of combustion reactions indicates that students in the KEG group had a 9.4 percentage point higher probability of being in the comprehensive understanding of collisions (COLEXP) sub-mode compared to students in the KOG group, after instruction. For clarity, we report the results of this analysis in a written form, including the respective estimates. However, we provide a full tabular summary of all ATT estimates in Table A8 in our SI.

Reaction start. In accordance with our hypotheses related to RQ2, our findings indicate that, for the start of reactions, the KEG group exhibits a significantly higher occupancy of the sub-mode COLEXP across both reaction types, suggesting that these students exhibit a deeper understanding of collision theory (ATT = 0.137 with $p = 0.03$ for the combustion reaction and 0.094 with $p = 0.04$ for the esterification reaction, respectively).

Reaction progress. We do not observe a significantly higher occupancy of the sub-mode COLEXP for any of the two reaction types when considering the reaction progress (ATT = −0.001 with $p = 0.904$ and 0.040 with $p = 0.15$, respectively). Furthermore, our findings indicate that in KEG, particularly for the esterification reaction, a macroscopic interpretation (MACRO) is significantly more prevalent (ATT = 0.256 with $p = 0.001$), whereas the interpretation focusing on bond breaking and formation (BONDS) is significantly less frequent (ATT = −0.203 with $p = 0.007$). This development is considered unfavorable, as MACRO opposes a submicroscopic understanding of reaction processes. Ordinal regression (part III) will shed further light on conditions for this development.

Reaction end. For complete combustion, no significant differences between KEG and KOG were observed regarding the end of reactions (see Table A8). Consistent with this, both groups showed similar transition patterns, with the limiting factor (LIMIT) displaying the largest gains or remaining stable over time (see Fig. 4 and 7). In esterification, however, KEG students showed a substantially higher likelihood of being classified in a dynamic understanding of equilibrium (DYNAMIC, ATT = 0.524, $p < 0.001$), whereas all other sub-modes were less represented. This pattern indicates differences between the groups primarily for reaction systems involving equilibrium.

Part III: effects on students' sub-modes in the post-condition

To further analyze conditions of conceptual development, we calculated stepwise prediction models of students' sub-modes in the post-condition. We successively incorporated general prior knowledge (last chemistry grade), specific prior knowledge (sub-modes in the pre-condition) and subject-related interest as predictor variables. In presenting the results, Fig. 8 summarizes the findings of all individual regressions. These findings are subsequently explained in more detail below. The full report of all regression models and parameter estimates are available in the appendix (Section F).

The comprehensive analysis within the framework of RQ3 reveals generally consisting findings across the established analytical unit, with specific variations depending on the combination of main mode and reaction example. In contrast to our usual structure along the three main modes (start, progress, end), we will present the findings visualized in Fig. 8 according to the stepwise introduction of predictors.

Specific prior knowledge. A detailed examination of the start of reaction of both reaction examples reveals that students possessing at least an initial understanding (INIT) in the pre-condition have significantly improved chances of reaching a higher conceptual sub-mode after the teaching unit. For instance, already possessing INIT increases the odds for the esterification reaction by a factor of 2.5 compared to no prior concepts (NOCONC) as the reference category). This finding supports the positive trend observed for INIT in the context of RQ1, as identified in the descriptive analysis of transitions between sub-modes. Furthermore, the next higher sub-mode of mutual attractions (ATTRAC) exerts an even stronger influence in the case of the esterification reaction. There is a significant advantage of ATTRAC over INIT in the pre-condition, resulting in a cumulative odds ratio of 5.44 for this reaction type.

At first glance, the direct effect of sub-modes in the pre-condition appears to be lower for the progress of the reaction. While there is no significant increase in the odds ratio when comparing the macroscopic understanding (MACRO) to the reference category of no prior concepts (NOCONC), students who already possess an initial understanding of bond breaking and formation (BONDS) have a significantly improved chance of reaching a higher conceptual sub-mode after the teaching unit, with a cumulative odds ratio of 3.63 compared to NOCONC. Interestingly, the best model fit includes interactions between sub-modes in the pre-condition and group membership. The analysis of the combustion reaction indicates a significant interaction effect of BONDS and group membership, suggesting that students in the KEG group who initially reasoned at the bond level had a substantially higher chance in reaching a higher conceptual sub-mode (odds ratio of 6.22). A closer examination of the esterification reaction revealed more pronounced group-dependent differences related to BONDS. The regression model showed a negative effect of pre-MACRO – the macroscopic interpretation of esterification reactions – for KEG students.

Notably, specific prior knowledge exhibits little to no importance in relation to the end of reactions. This challenges our expectations that specific prior knowledge would be an overall key predictor. Instead, group membership emerges as the most predictive factor for the end of reactions. While this effect was already evident in the differential DiD analysis for the esterification reaction through the calculated ATTs (which is reflected here by an odds ratio of 20.5 for the KEG group compared to the

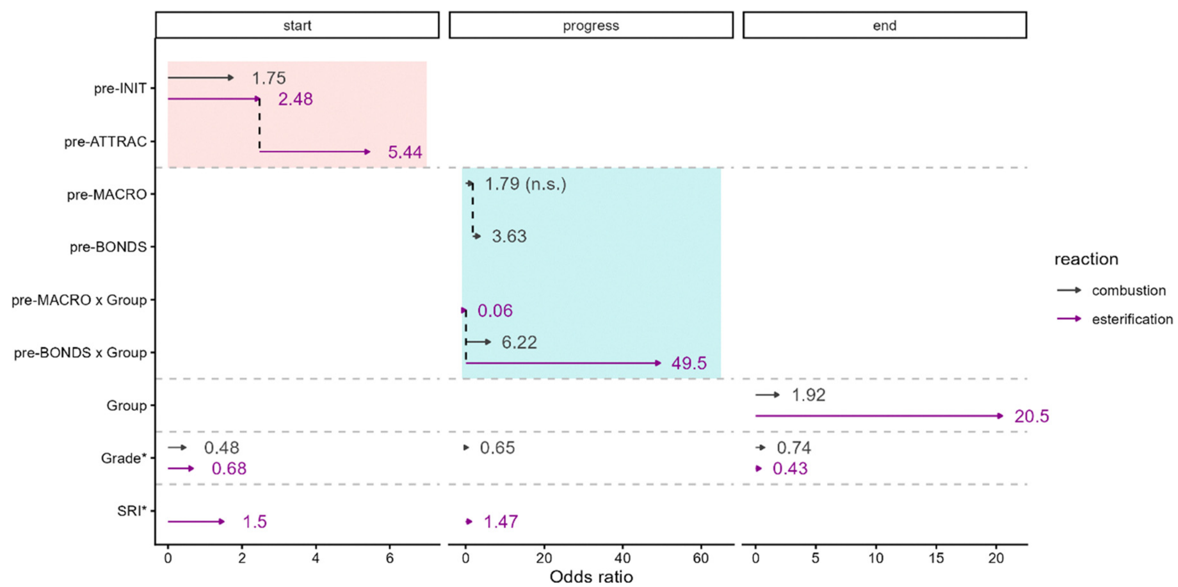

Fig. 8 Summary of effects on conceptual development in terms of Odds Ratios (ORs). Only significant effects are reported (*cf.* appendix). ORs above 1 indicate higher probabilities of reaching sub-modes with greater explanatory power after the teaching unit, whereas ORs below 1 indicate lower probabilities. Vertical dotted lines indicate relationships between consecutive sub-modes; in these cases, the OR values indicate the cumulative effect across the sequence of sub-modes in relation to NOCONC.

KOG group), a significant group advantage also manifests in the combustion reaction (but substantially lower, with an OR of 1.92). This advantage is not directly apparent from the ATTs but rather accumulates through the significant overall category shifts.

General prior knowledge. Across almost all combinations of conceptual mode and reaction example, the last chemistry grade, representing general prior knowledge, emerges as the most stable predictor. The ORs for this predictor range from 0.43 to 0.74, indicating that lower (*i.e.*, better) grades are associated with an increased likelihood of reaching a higher sub-mode category in the post-condition.

Subject-related interest. Subject-related interest (SRI), included as a covariate, showed significant effects only for esterification reactions. Specifically, higher SRI was associated with increased odds of reaching higher conceptual sub-modes for the start (OR = 1.50) and progress (OR = 1.47) of reactions. No significant effects were observed for the reaction end of esterification reactions or for any of the three modes in the case of combustion reactions.

Discussion

This study investigated the extent to which instruction on the topics, chemical kinetics and chemical equilibrium, can enhance learners' conceptual understanding of chemical reactions. We analyzed these conceptual transitions from multiple perspectives, considering (I) overall changes in the distribution of learners' conceptual sub-modes before and after instruction; (II) the differential impact of instruction on one *versus* both of these topic areas, identifying distinct learning gains and potential conceptual difficulties; and (III) the combined consideration of the isolated effects of theoretically relevant predictors.

Students' transitions on a conceptual landscape: a question of specific prior knowledge?

The results of analysis steps (I) and (III) indicate that both specific prior knowledge and general prior knowledge facilitated the cumulative development of conceptual understanding of chemical reactions. While learning opportunities related to chemical kinetics and chemical equilibrium led to significant shifts in learners' conceptual modes, our complementary analyses showed that students benefit from these learning opportunities in different ways. Specifically, students with higher prior knowledge – whether reflected in pre-condition sub-modes or chemistry grades – had in most cases a significantly higher likelihood of achieving conceptual growth. This finding supports the knowledge-is-power hypothesis (Hambrick and Engle, 2002; Etzel *et al.*, 2025), which posits that prior knowledge supports the effective use of learning opportunities. Contrary to our expectations, the relevance of specific prior knowledge did not differ as strongly from general prior knowledge. Additionally, including subject-related interest as a covariate strengthened the interpretation of prior knowledge effects by accounting for interest-related differences between students.

At the same time, the central contribution of our findings lies less in confirming the importance of prior knowledge – which is already well known from educational research – and more in demonstrating the value of assessing specific prior knowledge through conceptual sub-modes. Consistent with prior research, our analyses show that specific prior knowledge strongly predicts learning outcomes because conceptual modes build on one another (Brod, 2021; Edelsbrunner *et al.*, 2024). More importantly, the contrast coding partially revealed the cumulative structure of explanatory levels, thereby making visible how conceptual understanding develops across interconnected modes. For example, as an intended outcome of lower secondary education, bond breaking and reformation (BONDS) generally provided a productive foundation for further conceptual development. However, our findings also highlight group-related differences in the utility of this specific prior knowledge facet, as BONDS as a sub-mode in the pre-condition did not equally support all learners in advancing to higher conceptual modes. This was particularly evident in the KOG group, where BONDS supported transitions in esterification tasks less strongly. More specifically, students in KOG were unable to transfer their knowledge to ester-related tasks as their learning environment (see Table 1, KOG students only received instruction on lesson sets 1 and 2) did not explicitly provide opportunities to make such connections (Kehne, 2019).

Revealing this cumulative structure is of particular importance because it offers considerable diagnostic potential for identifying where students are progressing within the conceptual landscape and what conceptual support they may require. These implications for targeted conceptual support are discussed further in the implications section. At the same time, the sequential elaboration from lower to upper anchors of understanding highlighted in our findings demonstrates the potential of the present study to inform the design and validation of a future learning progression for upper secondary education. Overall, students who still exhibited a conceptual understanding at lower levels of reasoning by the end of lower secondary education were the least likely to benefit from new learning opportunities. This further underlines the importance of monitoring not only the quantity of students' understanding, but also their conceptual positioning and developmental trajectories.

Students' transitions on a conceptual landscape: a question of instruction?

In line with our expectations regarding effective time-on-task (Hattie, 2010), we found that learners in the KEG group demonstrated a deeper conceptual understanding regarding the reaction start in both reaction examples. However, these positive effects were not fully replicated for conceptualizing the reaction progress, where the macroscopic understanding and interpretation of reactions (MACRO) as pre-concept proved to be an obstacle for conceptual growth, particularly within the KEG group. Specifically, students with little prior conceptual knowledge (NOCONC) were more likely to transition into MACRO as an outcome, and those who started at this level were more likely to remain. This suggests a somewhat stabilizing effect of macroscopic reasoning. A more differentiated perspective reveals that

KEG learners who entered the learning environment and already possessed a more sophisticated concept of bond breaking and formation (BONDS) were somewhat protected from regressing at a macroscopic level of reasoning. A critical examination of the instructional materials and contexts suggests that the contextualization of the equilibrium concept within an aroma compound synthesis setting (see Table 1) – which frequently emphasized reaction yield, concentration trends, and concentration calculations – may have reinforced a macroscopic focus, particularly for learners who had not yet developed a submicroscopic understanding of the esterification reaction prior to the unit. With regard to developing a learning progression, this result supports the intertwined relation of instruction and learning progress as specific steps require specific instruction (Corcoran *et al.*, 2009), questions a strictly linear sequence (Sikorski and Hammer, 2017) and underlines that not every transition between possible steps is equal, but that specific intermediate conceptions (in this case MACRO) might serve as a gatekeeper. While the unit included activities that explicitly targeted a submicroscopic view of the end of reactions and their dynamic nature (Lossjew and Bernholt, 2025), aroma synthesis as a context seems to have reinforced macroscopic reasoning. At this point, stronger decontextualization and scaffolding with regard to the activation of appropriate resources may be needed (Parchmann *et al.*, 2006, Pölloth *et al.*, 2023). As expected, we observed the most pronounced effect for conceptualizing the reaction end, where KEG learners showed superior competence and an improved ability to differentiate reaction systems as they did not incorrectly overgeneralize their knowledge of the dynamic equilibrium state. This differentiation underscores that a conceptual shift between complete and incomplete reactions (Van Driel *et al.*, 1998) generally requires explicit instruction and should be addressed even more explicitly in a revised version of the instructional material.

Limitations

On a content level, examples were limited to two typical reaction types from school chemistry education. Previous research has shown that reasoning about chemical reactions is influenced by the specific reaction example (Yan and Talanquer, 2015). While these two reactions were carefully selected to cover different mechanistic and conceptual challenges relevant to school-level chemistry, our findings cannot be fully generalized to broader competence development within the core concept of chemical reactions, particularly for other reaction types such as redox reactions or polymerization processes.

From a methodological perspective, assessing learners' conceptual modes through open-ended responses offers advantages over traditional multiple-choice assessments (Emden *et al.*, 2018 ; Walpuski and Celik, 2024), as it provides deeper insights into students' reasoning processes. However, the classification of modes may also be influenced by response length and linguistic expression. In this regard, supplementary cognitive interviews could help capture students' ideas and reasoning, particularly for those who may struggle to articulate their understanding.

Although many international curricula share substantial commonalities regarding the core concept of chemical reactions, the study was conducted primarily in schools located in Northern Germany. This regional focus represents a limitation with respect to the generalizability of the findings. Similar research approaches could also be applied in international contexts to investigate students' learning about chemical reactions.

Conclusions and implications

This study provides evidence that learning opportunities in a research-informed TLS on chemical kinetics and chemical equilibrium generally lead to positive shifts in learners' conceptual modes, supporting the idea that targeted instruction on these topics fosters conceptual progression when reasoning about chemical reactions. In addition to the effects of instruction, we could confirm the well-known role of prior knowledge in this specific learning process. Beyond its generally positive influence, the findings also provide clear indications of the cumulative structure of the core concept of chemical reaction beyond lower secondary education and suggest that learning may additionally be shaped by affective constructs such as interest. The development and validation of a more detailed learning progression, substantially informed by the present study but requiring additional, more detailed task formats, represent logical next steps toward achieving this goal. We discuss these and further implications in the following section.

Implications for teaching and learning

While the importance of prior knowledge as a key determinant of students' conceptual development is not a surprising finding in itself, this study particularly provided insights into the cumulative structure of the investigated conceptual sub-modes and how these can be developed through the targeted activation of prior knowledge as well as instruction focusing on broader conceptual components (chemical kinetics and equilibrium). Uncovering these structural relationships opens diagnostic potential by enabling a more differentiated identification of students' conceptual starting points and learning pathways. We therefore argue for leveraging the diagnostic potential of digitally supported learning environments to assess students' conceptual understanding prior to entering new instructional units and to address identified conceptual gaps through targeted activities. These adaptations based on pre-diagnostic activities are also referred to as macro-adaptations. In our appendix, we further elaborate on these considerations by providing concrete design implications (Fig. A2). In small learning groups, teachers can already use the assessment instrument at the transition from lower to upper secondary education to evaluate specific goals of conceptual understanding in depth and to inform subsequent instructional planning. To our knowledge, at least in Germany, no systematic monitoring currently takes place at such educational transitions. Instead, responsibility largely lies with individual teachers. The proposed approach can support teachers in this diagnostic task. However, open-ended questions become difficult to implement with larger numbers of students. We briefly discuss this difficulty as part of the future research section. Beyond the macro-adaptations discussed here, digitally supported learning environments may also enable micro-adaptations, that is, task-level adaptations based on students' ongoing learning processes. This perspective was not the focus of the present study and would require further analyses at the task level to better support learners in conceptually critical tasks (*e.g.*, Schumacher and Stern, 2023). Likewise, identifying which tasks are particularly important for conceptual growth would require additional analyses (*e.g.*, Wyrwich *et al.*, 2025).

Implications for research in conceptual development

The assessment and analysis strategy applied in this study provides a valuable methodological framework for investigating students' conceptual development within the core concept of CR that could be extended to other questions of conceptual growth. It allows for a structured evaluation of whether learners have reached the learning objectives of lower secondary chemistry education, while also identifying conceptual transitions and reasons for divergent pathways. A key strength of this approach is its three-step design, which enables an exploration of conceptual growth from multiple perspectives. Our approach, thus, represents a first step towards the development of a learning progression by substantiating hypothetical pathways (*i.e.* theoretical learning progression) with empirical data and thereby preparing the ground for further LP-related analyses (*e.g.* Hadenfeldt *et al.*, 2016; Emden *et al.*, 2018).

The present study primarily focused on the mechanistic level conceptualized by Yan and Talanquer (2015), as the learning opportunities did not explicitly address causality-related reasoning regarding why chemical reactions occur. More complex structural-energetic reasoning (*e.g.*, Asmussen *et al.*, 2023; Braun *et al.*, 2024) was likewise beyond the scope of the target educational level. Future research could therefore investigate how learners integrate energetic considerations into mechanistic reasoning to further elaborate a learning progression extending towards university chemistry learning.

With regard to the structure of such an LP, we formulated "developmental statements" for upper secondary education based on our findings. These statements are provided in the appendix (Section I). The six statements outline how students are expected to progress in explaining matter, particle interactions, and the resulting course of chemical reactions, including how these processes are shaped by features of the reaction system. They are intended to inform further research towards the design and empirical investigation of an LP on chemical reactions in upper secondary education.

From a diagnostic perspective, evaluating complex student responses in large learning groups represents a considerable challenge for teachers. Based on the findings of our study, AI-based approaches for analyzing students' free-text responses therefore appear to be a logical next step, as they may offer promising opportunities to identify diagnostically relevant knowledge elements and support teachers' diagnostic work (*e.g.*, Gombert *et al.*, 2023; Bernholt *et al.*, 2025).

Conflicts of interest

There are no conflicts to declare.

Data availability

The data supporting this article have been included as part of the supplementary information (SI). Supplementary information is available. See DOI: https://doi.org/10.1039/d6rp00153j.

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Notes and references

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