Exploring processes and resources for problem solving at the crossroads between chemistry and mathematics

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Abstract

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Problem solving at the crossroads between chemistry and mathematics presents significant challenges for students at all levels of education. This licentiate thesis aims to enhance our understanding of such problem solving, with a focus on how university students approach problems in the context of chemical kinetics. The thesis is based on two papers. The video data analysed in these papers were collected from problem-solving sessions where second-year chemistry students worked in pairs to solve tasks centred around a key concept in chemical kinetics. The first paper aimed to develop a framework suitable for analysing problem solving at the interface of chemistry and mathematics. Deductive and inductive analysis of the collected video data resulted in *the extended mathematical modelling cycle (MMC)*. This empirically derived framework offers a fine-grained picture of the processes and resources at play during problem solving in chemical kinetics, suggesting that students: (1) engage in a range of (sub)processes beyond those typically outlined in the classical MMC; and (2) employ extra-mathematical resources (EMRs) in all stages of the MMC. The EMRs can be divided into *chemical* and *other resources*. While chemical resources are essential in translating chemical information into mathematical relationships, they also play a crucial role during mathematical work, offering guidance to the mathematical operations. The purpose of the second paper was to further characterise the nature and roles of *other resources*. Findings suggest that *other resources* can be divided into: implicit models of results, explicit examples from experience, and superficial procedural resources. Analysing their roles in problem solving revealed that implicit models primarily influence students' ideas of *where they are going*, while explicit examples and superficial procedural resources provide a basis of strategies for *how to get there*.

Keywords: Chemistry education research, mathematics education research, mathematical modelling, problem solving, chemical kinetics, metacognition, tertiary education, resources framework

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To my grandmother
致我的外婆

List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I. Ye, S., Elmgren, M., Jacobson, M., Ho, F.M. (2024) *How much is just maths?* Investigating problem solving in chemical kinetics at the interface of chemistry and mathematics through the development of an extended mathematical modelling cycle. *Chemistry Education Research and Practice, 25*(1), 242–265.

   Author's contribution: I conceptualised and designed the study in collaboration with my co-authors. I collected and transcribed the video data. Me and F.M.H. carried out data analysis to develop our coding scheme and the analytical framework used in the study. Note that this involved an iterative process where the analysis was continually discussed between all authors of the paper. I came up with, and created, *trajectories*, as a way to visualise our data and enhance the depth of our analysis. I wrote the initial draft of the manuscript, which then underwent review and editing by both me and my co-authors. The finalisation of the paper was a collective effort involving all authors.

II. Ye, S., Elmgren, M., Jacobson, M., Ho, F.M. (2024) More than numbers and molecules – exploring the nature and roles of non-disciplinary resources during problem solving in chemical kinetics. *Manuscript.*

   Author's contribution: I conceptualised and designed the study in collaboration with my co-authors. I collected and transcribed the video data. I carried out data analysis to develop an initial coding scheme. Note that this involved an iterative process where the analysis was continually discussed between all authors of the paper. I wrote the initial draft of the manuscript, which then underwent review and editing by the whole team. The finalisation of the paper was a collective effort involving all authors.

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Supporting work

Conference presentations

Ye, S., Elmgren, M., Jacobsson, M. & Ho, F.M. (2023). University students' reasoning and problem solving at the interface of chemistry and mathematics. In *2023 Meeting of Chemistry Education Research and Practice Gordon Research Conference,* Lewiston (ME), United States, July 9-14 [poster]

Ye, S., Elmgren, M., Jacobsson, M. & Ho, F.M. (2023). University students' reasoning and problem solving at the interface of chemistry and mathematics. In *2023 Meeting of Chemistry Education Research and Practice Gordon Research Seminar,* Lewiston (ME), United States, July 8-9 [oral presentation]

Ye, S., Elmgren, M., Jacobsson, M. & Ho, F.M. (2022). University students' reasoning and problem solving at the interface of chemistry and mathematics. In *6th PhD Chemistry Miniconference,* Uppsala, Sweden, September 26th [oral presentation, best oral presentation award]

Ye, S., Elmgren, M., Jacobsson, M. & Ho, F.M. (2022). University students' reasoning and problem solving at the interface of chemistry and mathematics. In *26th IUPAC International Conference on Chemistry Education,* Cape Town, South Africa, July 18-22 [oral presentation]

Contents

Notes for the reader

The use of language

For the majority of this thesis, I will use the singular pronoun ‘I’ to convey that the work presented herein reflects my own perspectives and ideas.

However, in Chapter 6, where I present overviews of my two papers, I will instead employ the collective pronoun ‘we.’ This choice acknowledges that the research papers are the result of collaborative efforts between me and my co-authors.

Similarly, in Section 7.2, where I discuss the implications of my research for teaching, I use the pronoun ‘we’ in referring to the collective of educators that might benefit from my research.

Furthermore, whenever I mention the category of resources called *other resources*, I will italicise the name to avoid potential confusion. To illustrate what I mean, consider the difference between ‘another resource’ (referring to an additional resource) and ‘an *other resource*’ (referring to the specific group of resources called *other resources*).

The use of previous work

In certain sections of this thesis, I have reused text passages that originally appear in the two papers that constitute this thesis. Sections in which such reuse has occurred will be marked by Roman numerals indicating the corresponding paper.

TL;DR – recommended reading

For readers primarily interested in the specific details and findings directly related to my research, rather than the broader aspects of chemistry education research, this list serves as a compilation of recommended readings.

- Chapter 1: Introduction
- Section 2.1.3: Research methods in CER
- Section 2.2: Mathematics in chemistry and physics education

- Section 2.3: Situating my own research
- Section 3.1.4: The resources framework
- Section 3.3.3: The mathematical modelling cycle
- Section 3.5: Laying the theoretical framework
- Chapter 4: Research questions
- Section 5.2.1: Research participants
- Section 5.2.2.3: General method for data collection in my research studies
- Section 5.2.3.2: Developing coding schemes for my research studies
- Chapter 6: Results and discussion
- Chapter 7: Conclusions, implications for teaching, limitations and future directions

1 Introduction

> The central point of education is to teach people to think, to use their rational powers, to become better problem solvers.
>
> (Gagné, 1980, p. 85)

As highlighted by Gagné (1980), a core objective of education is to support students in advancing their problem-solving skills. While problem solving within a single subject, like mathematics, may already be challenging in its own right, the complexity grows when elements from additional subjects are introduced. This brings us to the central focus of this thesis: problem solving at the crossroads between chemistry and mathematics.

On a more general note, problem solving at the interface of mathematics and *other disciplines* is known to pose significant challenges to students across various fields, including science, engineering, and economics (Biza et al., 2016). Contrary to the notion that this issue stems primarily from students' inability to 'do maths', there is now ample evidence that suggests otherwise, proposing instead that there are steps beyond algorithmic mathematical manipulations that serve as hurdles along the way (Uhden et al., 2012).

Within science education research, a range of studies in biology education research (e.g. Hester et al., 2014; Tetaj & Viirman, 2023; Viirman & Nardi, 2019) and physics education research (e.g. Carli et al., 2020; Gupta et al., 2007; Tuminaro & Redish, 2004; Van den Eynde, 2021; Wilcox & Pollock, 2015) indicate that the issue is prevalent from upper secondary school to advanced university level studies. Though much less researched, the same trend can be found in chemistry education: students across a range of educational levels struggle to combine their knowledge in chemistry with their knowledge in mathematics. In the realm of chemistry education, *chemical kinetics* has been identified as a fruitful context for study (Bain et al., 2019; Bain & Towns, 2016). This area poses considerable difficulties for chemistry students, requiring them to leverage their knowledge in mathematics and in chemistry, to carry out translations and transitions between physical phenomena and mathematical representations, in order to describe complex, interdependent, and multivariate phenomena.

Naturally, this issue has been investigated from the perspective of mathematics education research (MER) as well. Within this field, problem solving that bridges mathematics with other disciplines has been approached through the lens of mathematical modelling: the bidirectional act of describing real-world phenomena in terms of mathematical relationships, and making sense of mathematical formalisms in physical contexts (Niss & Blum, 2020b), with numerous research efforts indicating that students' struggles reside not *within* the mathematical domain but rather in the translations between the mathematical and the non-mathematical domain.

As evident from the preceding passage, previous explorations into problem solving at the interface of mathematics and other disciplines have largely been addressed from the standpoint of one or the other. Pursuant to calls for interdisciplinary approaches (National Research Council, 2012), my research combines theoretical lenses from chemistry, physics, and mathematics education research, to explore how university students tackle problem solving at the crossroads between chemistry and mathematics, focusing initially on the context of chemical kinetics.

1.1 Who should read this thesis?

This thesis aims to transcend disciplinary boundaries, reaching out to readers from diverse backgrounds who share a common interest in education.

For scholars engaged in chemistry education research and the broader field of science education research, this work offers valuable insights into the teaching and learning of problem solving, placing particular emphasis on problem-solving activities that involve mathematical modelling of extra-mathematical phenomena. On this note, this thesis should also be interesting for scholars in mathematics education research. While chemistry and science education researchers may benefit from gaining insight into the mathematical dimension of mathematical modelling, mathematics education researchers can benefit from gaining a better understanding of the extra-mathematical dimension.

For students, teachers, chemists and others, my hope is for Chapter 2 to serve as an introduction to the realm of chemistry education research.

1.2 Purpose and structure of the thesis

The overarching goal of my entire PhD project is to gain a better understanding of how university students tackle problems at the interface of chemistry and mathematics. What steps are involved in the problem-solving process? What are the characteristics of these steps? Where in the problem-solving process do students encounter challenges, and how do they overcome them?

This licentiate thesis serves as a presentation and discussion of what we have observed so far. The findings presented here originate from two studies exploring how students' knowledge and conceptual understanding of chemistry influence their use of mathematics when solving problems in chemical kinetics. The thesis follows the structure outlined below.

In **Chapter 1** (this chapter), I provide a brief overview of the thesis, outlining its relevance, contributions and purpose.

Chapter 2 is the literature review. Here, I describe previous research relevant to my studies. The purpose of this chapter is to offer the reader context for the questions posed, and the answers provided, in the thesis.

In **Chapter 3**, I present the theoretical framework of the thesis. That is, which theories, analytical frameworks and concepts that have guided the inquiry of my research questions so far, including how so.

Chapter 4 outlines the research questions discussed in this thesis, including the specific research questions addressed in each individual manuscript and study.

Chapter 5 concerns the methodology of the thesis. In this chapter, I connect certain aspects and assumptions of my theoretical framework to the research design, describing and motivating the chosen method for data collection and the general analytical approach. This chapter also discusses precautions taken to establish trustworthiness and reliability. The chapter ends with an account of the ethical considerations taken in this thesis.

Together, chapters 1-5 constitute the conceptual framework of my thesis. It explains *why* this research topic is interesting to study and what contributions my research may bring. It situates my research in relation to the existing body of literature and provides a detailed explanation of the chosen methodology. The chapters that follow are dedicated to my own research project.

Chapter 6 provides an overview of the individual papers covered in this thesis, including details on the data analyses and findings.

Finally, in **Chapter 7**, I present a summary of the conclusions of the thesis, including their implications for teaching. The chapter concludes with a brief discussion of the limitations of the thesis and some of my current ideas for future work.

2 Literature review

The first part of this chapter introduces the reader to the field of chemistry education research (CER) by providing a brief overview of the development of CER, including the topical areas that chemistry education researchers are concerned with, current trends, and some methodologies and methods common to the field. The second part of the chapter covers previous research relevant to the focus of this thesis, i.e. research on the role of mathematics in chemistry and physics education. In the final section of this chapter, I outline the relevance of my own research in relation to previous work in CER[1].

2.1 Chemistry education research

The field of chemistry education research (CER) is concerned with the intricacies of teaching and learning chemistry, exploring *what* we should teach our chemistry students and *how* we should do it.

Alongside fields like physics education research (PER), biology education research (BER) and computing education research, it falls under the umbrella of discipline-based education research (DBER). DBER operates under the premise that effective educational strategies must be tailored to the distinctive needs and characteristics of the subject matter; learning chemistry presents its own set of challenges, and successful teaching methods in chemistry may not necessarily translate seamlessly to the teaching of other subjects.

Given that researchers in chemistry education are interested in how human beings *think about chemistry*, rather than in the chemical entities themselves, the theories and methods employed within CER differ significantly from those employed in more traditional chemistry research. To make sense of their data, scholars in CER need not only a deep understanding of chemistry, they also have to be familiar with theories and methods pertaining to educational psychology and cognitive science. I will delve deeper into such theories and methods in Section 3.1 and Section 2.1.3, respectively.

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[1] Note that *chemistry education research* and *computing education research* often share the same abbreviation. For the sake of clarity, I specify that in this thesis, CER exclusively refers to *chemistry* education research.

In compiling this part of the literature review (Section 2.1), I have drawn inspiration from and relied on the review by Cooper and Stowe titled *Chemistry Education Research – From Personal Empiricism to Evidence, Theory and Informed Practice* (2018). To frame their review, Cooper and Stowe utilised the three thematic questions below. This section will be structured in a similar manner.

(Q1) What should students know about chemistry and what should they be able to do with that knowledge?

(Q2) How will we know that students have developed a coherent and useful understanding of chemistry?

(Q3) What evidence do we have about how to help students develop a deep and robust understanding of chemistry?

Before proceeding, I would like to make two remarks.

Firstly, a substantial amount of the CER literature has been, and is still, generated by authors based in the United States. While there are active chemistry education researchers on other continents as well, the majority of peer-reviewed work is conducted in North American settings. Since studies in CER seldom claim generalisability (a trait of qualitative research that will be further discussed in Section 2.1.3), this geographical concentration does not significantly impact the field's rigor. Nevertheless, it is important to be aware of the current geographical distribution of CER.

Secondly, this literature review does not account for investigations into pre-college chemistry education or CER focusing on laboratory work and the affective domain. I have deliberately chosen to omit these topics from this review as they fall outside the current scope of my thesis. For those interested in learning more about the research efforts within CER concerning laboratory work and the affective domain, I recommend recent reviews by Agustian et al. (2017, 2022; laboratory work), Seery et al. (2024; laboratory work) and Flaherty (2020; affective domain). In addition, readers interested in research on pre-college chemistry education might find the recent collection compiled by JCE useful (see Holme, 2023b, for a guide to this collection).

2.1.1 The development of CER

The *Journal of Chemical Education (JCE)* released its inaugural issue on the 1st of January 1924, almost exactly a hundred years ago. The anniversary was celebrated throughout 2023 by a series of virtual collections, showcasing influential works from the past century (published in the JCE) covering CER as well as topics such as the teaching of physical chemistry, inorganic chemistry, organic chemistry, biochemistry, analytical chemistry, high school chemistry and public outreach (see Holme, 2023c, for a complete list).

Although chemistry instructors have most certainly grappled with the question of how to teach chemistry for much longer, the late 1800s is generally regarded as the beginning of CER's history. The development of CER can be divided into two main periods, with Period I spanning from 1880 to 1960 and Period II beginning in the late 1960s. The subsequent sections provide brief overviews of these periods, before delving into some topical areas of CER, including learning objectives, assessment, teaching strategies, and curriculum design.

2.1.1.1 Period I: the era of 'personal empiricism'

During Period I, the literature on chemistry education mainly consisted of opinion pieces in which practitioners shared their personal teaching experiences and, quite astonishingly, the first issue of the JCE did not include a single reference. Cooper and Stowe (Cooper & Stowe, 2018) refer to this period as an 'era of personal empiricism'.

For example, Mabery (1893) published a paper suggesting that *enthusiastic instructors make the most successful teachers*. While there might be some truth to this claim, seeing that enthusiastic instructors are likely to gain more attention and engagement from students, it is no guarantee for students actually learning more about chemistry; in fact, there is little evidence to support this idea (Cooper & Stowe, 2018).

It is worth noting that, during this era, the content of chemistry classes was dictated largely by industrial and agricultural needs. Thus, the primary focus of chemistry education was to produce technically skilled chemists rather than fostering a deep understanding of chemical phenomena. This resulted in an emphasis on the practical aspects of chemistry, and class material was descriptive rather than theoretical in nature.

The content of chemistry courses underwent a significant transformation with the release of *Chemistry: Principles and Properties* by Sienko and Plane (1957). The idea was to create a book where relevant and accurate theory was introduced prior to delving into practical descriptions, and the book was therefore assembled from primary chemistry literature. While this did indeed shift the focus of chemistry education from a practical to a more theoretical orientation, Sienko and Plane's method for selecting topics was rather unconventional: they used what they referred to as a 'nodometer system'. That is, if students found a certain topic so dull that they fell asleep during the lecture, the topic was deemed too vague and obscure to be included. Nevertheless, the book gained widespread popularity, leaving a lasting impact on the structure of modern chemistry textbooks (Cooper & Stowe, 2018).

Clearly, chemistry education researchers active during Period I were deeply concerned with what students should know and be able to do with what they know (Q1, p. 13). Although these early contributions to the literature on chemistry education may not align with contemporary research standards, they played a crucial role in disseminating practical knowledge and cultivating a sense of community among educators.

2.1.1.2 Period II: learning theories enter the stage

In the late 1960s, CER began its transformation into the rigorous research field that it is today. During this period, learning theories from educational psychology and cognitive science made their way into chemistry education (Cooper & Stowe, 2018; T. Holme, 2023a). Two scholars who played crucial roles in shaping this phase of CER's history were: George M. Bodner (1946-2021), who introduced constructivist ideas to the field (Bodner, 1986); and Alex Johnstone (1930-2017), who explored the specific challenges related to the teaching and learning of chemistry by drawing on theories from cognitive science, including information processing theory and cognitive load theory (Johnstone, 1991; Reid, 2021).

Constructivism is a learning theory which posits that learners come with pre-existing knowledge structures and that learning is a process where new knowledge is actively constructed in the mind of the learner (Schunk, 2020). The theory has its roots in the works of Jean Piaget and Lev Vygotsky who were both concerned with the psychological development in children. While Piaget focused primarily on cognitive aspects of children's development, Vygotsky was more interested in the impact of social and cultural factors. Their different focal points led to two branches of constructivism referred to as *cognitive* constructivism (Piaget, 2015; Piaget et al., 1985) and *social* constructivism (Vygotsky, 1978). Both of these theories are part of my theoretical framework and are further described in Section 3.1.2.

Grounded within a constructivist perspective, Ausubel (1963, 1968) introduced the notion of *meaningful learning*, defining it as a kind of learning where new knowledge is connected to existing knowledge. In order for meaningful learning to occur, the following three requirements must be met: (1) students must hold the appropriate prior knowledge to which the new knowledge can be connected; (2) the new knowledge must be perceived as relevant (meaningful) to the prior knowledge; and (3) students must actively choose to incorporate the new knowledge into their existing knowledge. Importantly, if one or more of these requirements is not met, students often turn to *rote learning*, i.e. a kind of learning where facts are memorised without any connection to existing knowledge structures.

Novak extended Ausubel's notion of meaningful learning by proposing that meaningful learning requires the integration of thinking, feeling and acting (Novak et al., 1984). That is, for learning to be meaningful, it has to take place across the cognitive domain (what is to be learned – thinking), the affective domain (the attitudes and motivations of the learner – feeling) and the psychomotor domain (the physical activities that accompany learning – acting).

To sum it up, scholars and practitioners who embrace the philosophy of constructivism conceptualise learning as the *active construction of knowledge*. While cognitive constructivists focus on the mental processes of knowledge construction, social constructivists are more concerned with how the construction of knowledge is influenced by cultural and social contexts. Meaningful learning describes the process of learning from a constructivist point of view, suggesting that learning becomes meaningful only when the new knowledge is intentionally linked to existing knowledge structures. A crucial component of meaningful learning is the added emphasis on students' agency; in recognising that students have the autonomy to choose whether or not to engage in learning (Ausubel's criterion 3), educators must design their teaching to resonate with students' ideas of what counts as meaningful (Ausubel's criterion 2). Essentially, these constructivist ideas all contribute to placing the student at the heart of the learning process – a sentiment underscored by Craig (1972), who proposed that the teaching and learning of chemistry would likely improve if teachers spent more time talking to their students and thus gain a better understanding of what students know and do not know.

In the early 1980s, Johnstone brought ideas from information processing theory into the realm of CER. Information processing theory sheds light on the cognitive load associated with learning, recognising that learners have limited working memory capacity and that the way information is presented can influence the efficiency of learning. Balancing cognitive load becomes crucial, ensuring that the learning environment is challenging enough to stimulate growth but not overwhelming to impede understanding (Schunk, 2020).

Johnstone proposed that learning chemistry is challenging because it requires thinking at multiple levels and that such 'multi-level thinking' introduced far too much complexity for novice learners (Johnstone, 1982).

He formalised these ideas in his seminal paper, *Why is science so difficult to learn? Things are seldom what they seem*, introducing *the chemistry triplet* (Figure 1), which illustrates the language of chemistry through three levels of representation: the macroscopic, the submicroscopic (or particulate) and the symbolic level (Johnstone, 1991). More specifically, chemists must connect macroscopic observations with events taking place at the submicroscopic (or particulate) level to truly understand chemical phenomena. Additionally, effective communication in chemistry demands an understanding of the symbolic representations that chemists use to describe macroscopic and submicroscopic events, such as formulae and mathematical relationships (Johnstone, 1991). The chemistry triplet is sometimes referred to as *Johnstone's triangle*. Today, it is widely recognised that this multi-level nature of chemistry poses substantial challenges for students in their efforts to learn the subject (K. S. Taber, 2013; Talanquer, 2011).

Essentially, the CER conducted during Period II had two primary foci: firstly, to identify what students should know (Q1, p. 13); and secondly, to generate evidence of how to best support students in developing a deep and robust understanding of chemical phenomena (Q3, p. 13), drawing on learning theories such as constructivism and information processing theory in addressing the latter.

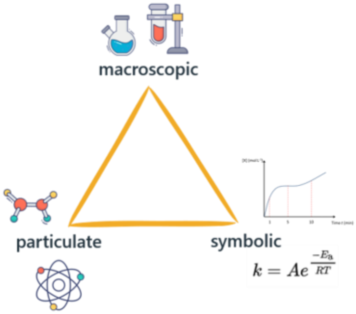


Figure 1. The chemistry triplet or Johnstone's triangle.

2.1.1.3 The impact of constructivism and the chemistry triplet on research concerning expertise and conceptual change

The transition to a more constructivist view on learning had significant implications for the research on expertise and conceptual change.

Expertise. According to constructivism, expert knowledge is organised in a coherent network, essentially mirroring the core principles of meaningful learning. With such a view of expert knowledge, the development of expertise can be seen as *the fostering of more expert-like knowledge structures* (Cooper & Stowe, 2018), thereby shifting the focal point from 'what' constitutes expert knowledge to 'how' it is constituted.

Johnstone asserts that experts in chemistry seamlessly connect and transition between all three levels of the chemistry triplet (Johnstone, 1991). That is, when observing a colour change in a reaction flask, an expert is able to connect this *macroscopic* change to a chemical reaction occurring at the *submicroscopic* level, and may describe the reaction using various *symbolic* representations; an expert effortlessly performs all these cognitive processes simultaneously. In contrast, a novice learner attempting to do the same is likely to experience working memory overload.

Cognitive load theory posits this difference between experts and novices to stem from variations in how they process information – more specifically, in how they consider, store and retrieve it. Research has shown that experts tend to consider and store knowledge in larger 'chunks' (Kozma & Russell, 1997), making it notably easier for them to retrieve the information when needed compared to novices. This phenomenon can be likened to experts and novices embarking on the same hike, with novices lacking an efficient system to carry all the required tools and equipment; even if a novice essentially has everything needed to complete the hike (or solve a given task), they might find it more challenging than experts as they lack an organised way to access and utilise their tools efficiently. In contrast, experts, with their well-structured ‘backpacks’ of knowledge, can navigate the task more seamlessly, leveraging the right tools at the right moments.

While the vertices of the chemistry triplet are concerned with the content of expertise knowledge (i.e. the ‘what’), it is the manner in which the content is related (i.e. the ‘how’) that foretells expertise. Hence, when it comes to expertise, both the tenets of constructivism and those of the chemistry triplet place greater emphasis on the *links* that connect knowledge rather than on the knowledge content itself.

A constructivist view of expertise asserts that educators need to provide students with learning opportunities where they can form connections between various pieces of knowledge. In other words, learning should be contextualised rather than taking place in an isolated, context-free, environment.

Conceptual change. During the 1970s and early 1980s, a significant portion of science education research revolved around students’ misconceptions (also referred to as preconceptions and alternative conceptions) of scientific phenomena (Cooper & Stowe, 2018). In the early days of exploring this topic, the prevailing notion was that misconceptions held by learners were distinct entities that could be replaced with more accurate ideas, and that the replacement process would take place if the learner was provided with a reason to reject their initial (mis)conception: a sort of ‘out with the old, in with the new’ mentality. This view had scholars within science education research dedicating considerable efforts to identify and document students’ misconceptions, generating *concept inventories* in various disciplines.

A concept inventory is an assessment tool specifically designed to evaluate students’ *conceptual* understanding of a particular subject. An example is the Chemistry Concepts Inventory (Mulford & Robinson, 2002), which is a multiple-choice test featuring questions about fundamental chemistry concepts typically introduced during high school and first-semester college chemistry courses. The purpose of concept inventories is to identify students’ alternative conceptions.

While these early efforts did indeed demonstrate a growing awareness of students’ entering the classroom with pre-existing knowledge, initial attempts in science education to guide students in replacing their misconceptions with corresponding correct ideas proved more challenging than anticipated (diSessa, 2014). In contemporary models of conceptual change, misconceptions are instead viewed as explicit manifestations of implicit cognitive structures: a learner’s (mis)conception of a given phenomenon represents only ‘the tip of the iceberg’, reflecting a larger network of knowledge. Such a view predicts the process of conceptual change to be far more complex than a simple exchange of one idea for another; the substitution must also account for the overall ecology, or coherence, of the existing knowledge structure.

In 1993, diSessa introduced his *Knowledge-in-Pieces (KiP)* model, suggesting that a learner's understanding of a concept is comprised of knowledge pieces smaller than the concept itself. He referred to these knowledge pieces as *phenomenological primitives (p-prims)*. The model emerged as a response to prevailing learning theories of conceptual change and intuitive physics, in which novices were portrayed as having a few coherent knowledge structures. diSessa criticised these views, arguing that they were bound to overestimate either the influence of a single element in setting the stage for all others, or the strength and coherency of the links holding a set of elements together. In contrast to these views, diSessa proposed the perspective of KiP, underscoring the dynamic nature of knowledge structures (Elby et al., 2001). It is worth noting that the KiP model does not refute the idea of coherence in novices' knowledge structures; instead, it posits that coherence is momentary, arising due to context-dependent activation rather than being predetermined and fixed. This conceptual shift challenged the notion of static representations of knowledge prevalent in earlier theories.

Other scholars within PER have since built on diSessa's ideas and *the resources framework* has emerged as one of the more influential modern models of conceptual change (Hammer et al., 2005; Redish, 2004). Similar to diSessa's KiP model, the resources framework posits that knowledge is constructed from small cognitive units, emphasising the dynamic nature of knowledge structures. However, within the resources framework, the cognitive units are referred to as *resources*. Viewing knowledge through this lens carries implications for several learning principles, including transfer and conceptual change. Rather than treating learned concepts and abilities as fixed entities that are either transferred or not, researchers within the resources tradition consider learners to possess various a range of resources that can be *activated* and employed in various ways depending on the context (Hammer et al., 2005). As such, this perspective offers a plausible explanation for how the same student might demonstrate different, and at times contradictory, reasoning and problem-solving approaches in response to a given setting; the student's perception of the context dictates which resources that are activated. The resources framework is part of my theoretical framework and will be discussed in greater detail in Section 3.1.4.

2.1.1.4 Learning objectives: What students should know about chemistry and be able to do with what they know

Since the very beginning of CER's history, scholars within the field have been concerned with the question of *what chemistry students should know and be able to do with what they know* (Q1, p. 13). As already mentioned, the answer to this question during the first half of the 20th century was largely shaped by industrial and agricultural needs. Two significant paradigm shifts occurred in the late 1950s and 1960s. To begin with, the content of chemistry courses shifted from a practical to a more theoretical focus. Next, the field of CER matured from primarily relying on anecdotal work to embracing evidence-based methods rooted in learning theories such as constructivism and information processing theory (Cooper & Stowe, 2018).

During the latter half of the 20th century, two crucial realisations brought about a shift in the approach to addressing Q1 (p. 13). Firstly, the CER community noticed that general chemistry courses had become both broad and superficial. Although students acquired knowledge across a wide range of topics, this knowledge was typically superficial: they learnt a little about a lot. Secondly, there was a growing awareness that not all students who enter a chemistry class are there to become chemists; in fact, chemistry classes often include aspiring engineers, doctors, teachers and more, and it is essential to address their interests as well (Cooper & Stowe, 2018; Osborne & Dillon, 2008). These realisations led to scholars in CER reconsidering *what students should know and be able to do with their knowledge*: if the objective of a chemistry course is not for every individual to become professional chemists, perhaps it is inappropriate for *expertise in chemistry* to be the sole criterion guiding the content covered in a chemistry course?

In the United States, this shift in perspective prompted the development of numerous guidelines aimed at defining what chemistry students should know based on their level of study and academic direction. For instance, Gillespie (1997) and Atkins (1999) independently introduced specific sets of ‘great ideas’: core chemical concepts serving as anchors for related sub-concepts, thus reflecting a view on the structure of expert knowledge in line with constructivist principles. Following the works of Gillespie and Atkins, various other guidelines were proposed, culminating in the Anchoring Concepts Content Map (ACCM) developed by *the American Chemical Society’s Exams Institute*. The ACCM stands as the most comprehensive and detailed list of what students should know after completing a chemistry course. A comparison of these guidelines can be found in Table 1 in the review by Cooper and Stowe (2018).

Since possessing a wealth of chemistry facts proves valuable only when one can apply that knowledge, the CER community is also concerned with the question of what chemistry students should be able to do with what they know. Such abilities are captured by the list of *scientific and engineering practices* compiled by *The National Research Council* (see Box 3 in Cooper & Stowe, 2018). Essentially, scientific and engineering practices correspond to what is commonly recognised as problem-solving skills. A more detailed discussion of problem solving (in general and in CER) is given in Section 3.2.

As a final remark on scientific and engineering practices, I emphasise that the aspect of *planning and executing investigations* holds a particularly important role in chemistry education, forming the rationale for laboratory work as part of the chemistry curriculum. While this topic is not extensively covered in this licentiate thesis review, it has been thoroughly reviewed elsewhere (Agustian et al., 2022; Seery et al., 2024).

2.1.1.5 Assessment: Ensuring that students have developed a coherent and useful understanding of chemistry

Identifying what students should know holds limited value unless educators have reliable methods to confirm that students have truly acquired that which they are expected to know. This constitutes a topical area within CER, where scholars dedicate their research efforts to the development of instruments and tools for assessment, thus aiming to address the question of how we can know that students have developed a coherent and useful understanding of chemistry (Q2, p. 13; Cooper & Stowe, 2018).

An early example of such efforts is found in the work of Cornog and Colbert, who, in 1924, surveyed faculty from 27 different institutions to explore what they believed chemistry students should know after completing a course in general chemistry. The aim of the study was to gain a better understanding of the alignment (or misalignment) between teachers' intended learning objectives, the course material used to convey these objectives, and the content assessed in the examinations. Despite most instructors expressing an intended focus on the theoretical aspects of chemistry, it was uncommon for the corresponding course material and examinations to reinforce such a perspective. A particularly valuable insight from Cornog and Colbert's study (1924), still relevant in chemistry education today, came from their observation that examinations significantly influence how students allocate their study efforts. Thus, a well-crafted exam serves not only as an instrument for educators to evaluate students' understanding of chemistry but also as a guide for students, sending them a powerful message about what truly matters in their studies.

In the United States, chemistry assessments are typically categorised into three groups: exams developed by the *American Chemical Society's Exams Institute*, exams based on concept inventories (Section 2.1.1.3), and other assessments found in the literature (Cooper & Stowe, 2018). For an assessment tool to be considered valid, the National Research Council recommends that the assessment process follows the method outlined by the *assessment triangle*. Thus, the assessment process should include: (1) a domain-specific model of student cognition and learning, (2) the kinds of observations that are expected to provide evidence of students' competencies, and (3) an interpretation process for making sense of the evidence (National Research Council, 2001). Further details are provided in the review by Cooper and Stowe (Cooper & Stowe, 2018). However, readers should be aware that Cooper and Stowe's review primarily reflects a North American context.

In European countries, there have been fewer efforts in drafting such nationwide guidelines for chemistry assessments at the university level, prompting a need for further research in this area (Osborne & Dillon, 2008). Nevertheless, there are examples of standardised tests at the school level.

For instance, *The Swedish National Agency for Education* (*Skolverket* in Swedish) organises *national tests* during primary school (3rd, 6th and 9th grade) and high school. In primary school, national tests typically cover a set of core subjects including Swedish, English and mathematics, with an additional test in one social science subject and one natural science subject in the 9th grade. At the high school level, it is mandatory for all teachers to conduct national tests in Swedish and English. In addition, teachers can choose whether or not to administer national tests in chemistry, biology, physics, history and in one of the ‘modern languages’, i.e. French, Spanish or German (Skolverket, 2024).

2.1.1.6 Teaching strategies: Evidence about how to help students develop a deep and robust understanding of chemistry

The aforementioned topical areas of CER concern the objectives of chemistry education (Q1, p. 13) and the development of methods for assessing the attainment of those objectives (Q2, p. 13). Another important question is how we, as educators, can support our students in achieving these educational goals. In this section, I aim to provide the reader with a brief introduction to the evidence produced by the CER community regarding effective strategies for fostering the development of a robust understanding of chemistry among students (Q3, p. 13). This topical area can be divided into three sub-areas.

Student engagement. One such sub-area is that concerned with *student engagement*. That is, the degree to which students demonstrate interest in, attend to, and participate in a learning activity. While student engagement is undoubtedly influenced by individual differences among students, external factors also play a significant role. An example of such an external factor is the learning environment, which partly depends on the chosen pedagogical approach (Cooper & Stowe, 2018). Thus, the study of student engagement is closely intertwined with the study of pedagogical approaches and their impact on students’ learning.

In recent years, *active learning* has emerged as a crucial component of modern teaching methods. Aligned with constructivist ideas, these methods encourage students to actively participate in their own learning journeys, as opposed to the more traditional teaching format with students acting merely as passive recipients of knowledge. Active learning can be implemented through a variety of activities, for example by: incorporating moments for students to ‘think-pair-share’ during class; integrating formative assessments at the end of a learning activity; and adopting a flipped classroom approach (Freeman et al., 2014).

Process Oriented Guided Inquiry Learning (POGIL) is a student-centred teaching strategy, rooted in the principles of active learning and constructivism, that has gained particular traction in STEM education. In a typical POGIL setting, students collaborate in small groups to tackle pre-designed problems, with the instructor serving as a facilitator rather than a source of information. As the name suggests, the goal of a POGIL activity is to *guide* students through the inquiry of some part of the course content. The first two terms, *process oriented*, underscore that POGIL activities foster not only the understanding of course-specific material, but also cultivate more general *process skills*, such as critical thinking, problem solving, metacognition, teamwork, information processing and communication (Rodriguez, Hunter, et al., 2020).

Visualisations and representations. Another sub-area within the broader topic of optimising strategies for teaching chemistry focuses on the use of various tools to visualise and represent chemical phenomena. The complex language of chemistry, captured by the chemistry triplet (Figure 1), places particular importance on a learner's ability to make sense of, and utilise, visualisations and representations. The importance of this matter is evident in the literature, with numerous publications, themed issues, and books delving into the specific challenges and solutions pertaining to the subject. Some noteworthy examples include: a themed issue on *Visualisations and Representations in Chemistry Education* published by the journal *Chemistry Education Research and Practice* (see Kelly & Akaygun, 2019, for a complete guide); the book *Multiple Representations in Chemistry* (Gilbert & Treagust, 2009); and a recent thesis from the Linnaeus University titled *Exploring the Role That Visual Representations Play When Teaching and Learning Chemical Bonding* (Patron, 2022).

The sub-area of visualisations and representations comprises two major research strands: (1) investigating how students use and interpret existing representations of molecules and molecular behaviour; and (2) developing novel ways to visualise and represent molecules and molecular behaviour. Note that visualisations and representations encompass not only 3D models of molecules but also chemical formulae, various diagrams, spectra, and more.

Unsurprisingly, a considerable amount of the research conducted within this sub-area focuses on the teaching and learning of organic chemistry – a subject requiring students to understand the underlying molecular events that govern organic reactions and to make sense of a rich symbolic language (e.g. molecular structures, reaction mechanisms, electron-pushing arrows).

The Graulich Group at Giessen University has made substantial contributions to the branch of CER concerned with organic chemistry, using eye-tracking technology to advance our understanding of how students interact with visualisations and the multitude of representations employed in organic chemistry education (Rodemer et al., 2020, 2021). For those interested in the essentials of eye-tracking technology and how it may be employed in CER, I refer to the book by Sweeder and colleagues published in 2019.

Instructional technology. A third sub-area of teaching strategies focuses on the usefulness of digital tools and multimedia and how to optimise their integration into chemistry education (Cooper & Stowe, 2018). Naturally, this research area is closely related to that of visualisations and representations; after all, a primary objective of utilising digital tools and multimedia is to visualise various representations of chemical phenomena (e.g. Ardac & Akaygun, 2004; Jones, 2013; Mayer, 2014). Such use of visualisations has been shown to enhance chemistry students' understanding of the relationship between macroscopic and particulate events.

An example of how a better understanding of the ways in which students interact with visualisations and representations can inform the development of teaching strategies is found in a recent study by Langner et al. (2022). In this study, researchers employed eye-tracking technology to assist pre-service teachers in reflecting on their future use of digital tools. More specifically, the participating pre-service teachers were asked to complete three assignments: (1) to design learning material incorporating various forms of multimedia; (2) to conduct a small-scale eye-tracking study, observing how students interacted with the designed learning material; and (3) reflect on how to purposefully design multimedia learning material.

The relevance of research on instructional technologies became particularly pronounced in response to the challenges posed by the global COVID-19 pandemic. Forcing schools and universities worldwide to swiftly transition from traditional on-site learning to online (distance) learning, the pandemic prompted a profound re-evaluation of the defining elements of effective teaching strategies (Talanquer et al., 2020). The sudden shift resulted in a wealth of publications offering valuable insights into effective strategies for implementing instructional technology in chemistry education. For instance, the *Journal of Chemical Education (JCE)* assembled a virtual collection of past publications containing material relevant to instructors transitioning to online teaching (Journal of Chemical Education, 2019). Additionally, the JCE released a special issue titled *Insights Gained While Teaching Chemistry in the Time of COVID-19* (Holme, 2020).

Yet another pivotal moment shaping our approach to teaching chemistry was the recent launch of ChatGPT. Surely, no teacher has escaped its impact on education. This topic will be further discussed in Section 2.1.2.3.

For educators seeking to expand their library of teaching strategies, Felix Ho at Uppsala University has carefully curated a guide to various relevant digital resources such as research journals, special themed issues and visualisation tools (Felix Ho, 2023).

2.1.1.7 Curriculum design: Ensuring that relevant findings from CER is effectively realised in the classroom

The previously mentioned topical areas are concerned with: (1) what students should know and be able to do with what they know, i.e. learning objectives; (2) how to make sure that the students have acquired that which they should know, i.e. assessment; and (3) evidence about how to support our students on their learning journeys, i.e. teaching strategies. The aim of curriculum design is to ensure that relevant findings from each of the aforementioned topical areas are effectively realised in the classroom. This can be achieved through the alignment of learning objectives, assessments and instructional strategies: an approach sometimes referred to as *constructive alignment* (Elmgren &

Henriksson, 2015). As neatly described by Cooper and Stowe, the purpose of curriculum design is to 'tie evidence to practice' (2018) .

2.1.2 Current trends and future directions in CER

In this section, I provide an overview of the contemporary landscape of CER. The section begins with a reflection on how insights from the global pandemic have sparked: (1) a re-evaluation of what chemistry students should know and be able to do (Q1, p. 13); and (2) a growing recognition of the fundamental role played by research on diversity, equity and inclusion (DEI) in advancing the field of CER. Following this, I discuss the impact of generative artificial intelligence (AI) on education: how it has prompted instructors worldwide to reconsider the construction of educational materials (Q2, p. 13); and how scholars within DBER are currently exploring the potential use of chatbots in the development of innovative teaching strategies (Q3, p. 13). Essentially, these sections aim to connect the ramifications and revelations of recent global changes to the aforementioned thematic questions (p. 13). Finally, the section concludes with a brief summary of promising avenues for further investigation.

2.1.2.1 Impact of the COVID-19 pandemic: preparing students for the challenges of tomorrow

The global upheaval caused by the COVID-19 pandemic prompted a profound re-evaluation of the overarching learning objectives of chemistry education, i.e. what chemistry students should know and be able to do with what they know (Talanquer et al., 2020). Although the pandemic showcased immense strength in the scientific apparatus, offering solutions through rapid progress in vaccine research and other related fields such as epidemiology and immunology, it also exposed societal inequities and a strong distrust towards science (Agustian, 2023; Wilson-Kennedy et al., 2022).

These insights catalysed a paradigm shift in science education, leading to a reassessment of its very purpose and the types of challenges it should prepare students for (Talanquer et al., 2020). The current consensus is that science education should: (1) cater a broader audience, aiming not only to produce scientists and engineers but also to foster scientifically literate citizens; and (2) strive to equip students with the knowledge and skills necessary to tackle problems that are authentic and relevant to the world we live in (Osborne & Dillon, 2008). Two distinct subsets of authentic problems are *real-world problems* and *wicked problems*.

Within the realm of education, *real-world problems* refer to challenges or issues that mirror the complexities of the world beyond the classroom. In contrast to decontextualised textbook problems and drills, addressing real-world problems typically requires students to model authentic scenarios, engage in critical thinking, conduct data analysis, make decisions, and more. In other words, real-world problems place a significant demand on students' overall problem-solving skills (Geiger et al., 2018).

A *wicked problem* shares similarities with a real-world problem but is distinguished by an even higher complexity. Wicked problems are ill-defined, intertwined and multifaceted in nature, making it difficult to pinpoint a specific source and, consequently, determine where efforts should be directed to address the issue. Moreover, wicked problems often involve numerous stakeholders and lack clear-cut solutions; such presence of conflicting interests and ethical dilemmas poses unique challenges for knowledge generation and resolution. Examples of wicked problems include the COVID-19 pandemic and climate change, both considered wicked problems due to their complex, interconnected natures, involving stakeholders across environmental, social, economic, and political dimensions (Agustian, 2023; Block et al., 2019).

Addressing real-world and wicked problems in education requires a shift in how we approach both research and practice, calling for collaboration across disciplines and sectors. Recommended pedagogical strategies include: *interdisciplinary learning,* encouraging students to integrate knowledge from diverse disciplines; placing an emphasis on *critical thinking* to equip students with the ability to analyse and interpret information critically; creating learning environments that foster *collaboration and cooperative problem solving*; offering opportunities for *experiential learning,* such as internships and project-based activities, to provide students with hands-on experiences; and incorporating principles of *systems thinking* into the curriculum to support students in developing an understanding of complex phenomena as integrated systems rather than isolated components (Orgill et al., 2019). Prominent scholars in science education have also underscored the role of *out-of-school activities* in preparing students to tackle authentic problems, e.g. museum visits, science clubs and community service (Achiam et al., 2021).

In addition to these pedagogical strategies, it is important that educators work to cultivate skills and abilities pertaining to the affective domain. For instance, emotional intelligence and empathy are crucial for the effective communication between individuals of diverse backgrounds and interests. Moreover, affective abilities are essential for students in reflecting on the ethical implications of their decisions and actions. Finally, it is imperative that educators worldwide support their students in adopting mindsets of *continuous learning and adaptation*, thus recognising that addressing wicked problems requires ongoing reflection, learning, and adjustment (Achiam et al., 2021).

Altogether, these pedagogical strategies and learning objectives all serve to create learning environments that mimic the uncertainties and interconnectedness of real-world and wicked problems.

2.1.2.2 Impact of COVID-19 pandemic: amplifying the significance of research on diversity, equity and inclusion

Over the past two decades, there has been a notable increase in research efforts focused on diversity, equity, and inclusion (DEI) in STEM education. This surge gained momentum in the aftermath of the global COVID-19 pandemic, which further exposed and magnified already existing inequities embedded within our educational systems (Barnett, 2020; Sweeder et al., 2023; Wilson-Kennedy et al., 2022). Extending beyond the individual scopes of the aforementioned thematic questions (p. 13), this topical area permeates all facets of chemistry education.

Essentially, education researchers concerned with DEI seek to identify and address disparities in access, opportunities, and outcomes within educational systems. With the aim of ensuring that every student experiences an inclusive and equitable learning environment, scholars in this domain are dedicated to the exploration of strategies to foster cultural competence among educators, the development of inclusive curricula, and the implementation of policies that cultivate an educational landscape where diversity is celebrated, equity is upheld, and inclusion is considered a cornerstone of learning and growth. To conclude, the goal of DEI research is to create educational settings that empower *all* students to thrive, regardless of their cultural, social, or individual differences (Kassam, 2022; Wilson-Kennedy et al., 2022).

Within CER, a predominant focus of DEI efforts has been to increase the representation and academic achievements of chemistry students coming from historically marginalised groups (Ryu et al., 2021). Encouraging the CER community to ‘dream bigger’ and go beyond the study of numerical metrics, Ryu et al. (2021) propose three future directions of DEI research in CER: investigating less-explored contexts; embracing holistic approaches to program reform, e.g. by considering reform across institutional levels; and advocating for curricular reform to be justice- and relevance-oriented.

For readers interested in learning more about the current state of DEI in chemistry education and CER, I refer to a recent special issue on the topic published by the JCE (see Wilson-Kennedy et al., 2022, for an introduction).

2.1.2.3 Generative artificial intelligence and education

ChatGPT is a type of generative artificial intelligence (AI) belonging to the family of large language models (LLMs), designed to generate human-like text based on the input it receives. The acronym GPT stands for *Generative Pre-trained Transformer*, signifying that it: (1) can *generate* new content, rather than merely recognising or classifying already existing data; (2) has undergone *prior training* on a large dataset to learn how to predict the next word in a sequence based on the context revealed by previous words; and (3) builds on a neural network architecture particularly effective for tasks related to natural language processing (ChatGPT, OpenAI, 2023).

Initially, the introduction of ChatGPT perplexed educators worldwide, having them grapple with the challenges of creating ‘ChatGPT-proof’ assignments and examinations: exercises asking students to define or explain various concepts and terms seemed almost futile in the face of the powerful chatbot. This does not imply that teachers were unfamiliar with alternative approaches to testing students’ knowledge; however, it underscores that the emergence of ChatGPT and other chatbots emphasised the need to reconsider conventional methods for constructing and evaluating assessments (Polverini & Gregorcic, 2024; Watts et al., 2023).

As educators and researchers have become more acquainted with ChatGPT, the initial uncertainty has faded, allowing for new perspectives. Instead of viewing these technological advancements as potential sources of educational pitfalls, scholars are now exploring how to incorporate ChatGPT, and other types of generative AI, into teaching strategies, harnessing their potential as valuable educational aids.

Several publications on the role of generative AI in education are already available in the science education literature. Within CER, Watts et al. (2023) recently published an article reporting on a comparison of student and chatbot responses to a writing-to-learn assignment focused on mechanistic reasoning in organic chemistry. They produced responses from three different generative AIs (ChatGPT-3.5, ChatGPT-4, and Bard) and found that none of the chatbots were able to engage in mechanistic reasoning at the same level as students. In PER, a recent paper from Polverini and Gregorcic (2024) contributes with a comprehensive introduction to educators and scholars interested in the use of LLMs in physics education.

2.1.2.4 Summary and future directions of CER

Looking ahead, there are several promising avenues for future research in CER, many of which have already been discussed in the preceding sections. In the forthcoming years, scholars within the CER community will continue to, among other things:

- re-evaluate what chemistry students should know and be able to do with their knowledge;
- implement teaching strategies to better prepare students for the complex problems of tomorrow;
- promote the integration of DEI values in both chemistry education research and practice;
- investigate how to optimise the use of technology for the advancement of chemistry education as well as CER.

Another significant future direction involves the exploration of upper-level chemistry courses. Given the predominant focus of existing CER literature on studies conducted in the context of introductory-level courses, scholars are encouraged to delve into the particular challenges of teaching and learning more advanced chemistry topics.

2.1.3 Research methods in CER

Before delving into some common research methods in CER, I would to make a remark regarding the difference between a *method* and a *methodology*. While a research *method* refers to the specific tools and techniques used to collect and analyse the data, i.e. the things you do to carry out your research, a research *methodology* can be understood as the rationale for using a given set of research methods (Cohen et al., 2018).

Each research methodology comes with certain strengths and limitations, offering researchers a lens through which they can approach their research questions. The choice of methodology ultimately depends on the objectives of the research project, the nature of the phenomenon under investigation, and the desired depth or breadth of understanding. Together with the theoretical framework, the methodology guides the research design, including which methods to use. Examples of research *methodologies* include naturalistic, ethnographic, quantitative, grounded theory, qualitative, and post-qualitative research (Bunce & Cole, 2008; Cohen et al., 2018).

In CER, most scholars adopt a quantitative, qualitative or mixed-methods approach (Creswell & Creswell, 2022). Herein, I give a brief overview of these three methodologies, including examples of corresponding research methods.

The methodology employed to explore the research questions of this thesis falls within the qualitative research paradigm and is outlined in Chapter 5.

2.1.3.1 Quantitative research

Quantitative research *methodologies* involve the systematic collection and analysis of numerical data to identify patterns and relationships of statistical significance. In other words, researchers employing a quantitative research methodology utilise various statistical tools and instruments to address their research questions.

In educational research, quantitative *methods* typically entail data collection through surveys, polls or controlled experiments, aiming to generate large datasets that can undergo statistical analysis. These methods are particularly well-suited for exploring the prevalence of specific trends, investigating correlation among variables and assessing the effectiveness of interventions. For example, a quantitative research study may involve the researcher manipulating independent variables to observe their effect on dependent variables in a controlled setting, thereby facilitating the establishment of cause-and-effect relationships (Creswell & Creswell, 2022).

2.1.3.2 Qualitative research

Qualitative research *methodologies* are explorative in nature, catering to researchers seeking to understand the context, meaning, and underlying mechanisms of the studied phenomenon. Thus, qualitative research studies are often conducted with relatively small cohorts as compared to quantitative studies. In educational research, qualitative methodologies focus on individuals' subjective experiences of education, including cognitive, affective, psychomotor and social aspects (Erickson, 2012).

Common qualitative *methods* for data collection are interviews and observational studies. The research data is typically non-numerical (e.g. video, audio or text) and can be subjected to various forms of qualitative data analysis, such as content analysis, thematic analysis and/or discourse analysis. Qualitative research methods are suitable for exploring complex, context-dependent research questions (Cohen et al., 2018; Erickson, 2012).

2.1.3.3 Mixed-methods research

Conclusions derived from quantitative research studies are often generalisable to a larger population. This contrasts with qualitative research studies, which provide in-depth insights into specific contexts or individuals, offering findings applicable to similar settings rather than broader generalisation. To bridge the gap between *breadth* and *depth*, it may in some cases be appropriate to adopt a *mixed-methods* approach. A mixed-methods research design combines quantitative and qualitative methods of data collection and analysis within a single study (Towns, 2008).

For example, the effectiveness of an educational intervention can be tested by comparing exam scores between students who received the intervention and those who did not (quantitative data collection and analysis). While such a comparison can indicate whether the intervention was effective, it does not explain *why*. To delve into the *why*, we could interview a subset of students and analyse their responses to identify themes and patterns (qualitative data collection and analysis). In such way, a mixed-methods approach can provide insights into the effectiveness of an intervention as well as the underlying mechanisms that contribute to the effectiveness or lack thereof (Cooper & Stowe, 2018).

2.2 Mathematics in chemistry and physics education

2.2.1 The role of mathematics in physics education[I]

Over the past two decades, there has been a remarkable growth in the body of literature exploring the role of mathematics in scientific disciplines. Much of this work has focused on its role in physics education (Palmgren & Rasa, 2022; Pospiech et al., 2019). While traditionally, mathematics has been regarded primarily as a tool in physics, its role has lately been recognised to extend beyond these conventional notions, suggesting a twofold nature (Uhden et al., 2012).

In 2006, Redish emphasised that *using* mathematics in physics differs from simply *doing* mathematics. Building upon this idea, and a distinction introduced by Pietrocola (2008), Uhden et al. (2012) proposed that mathematics has two distinct roles in physics: a *structural* role and a *technical* role. The technical role of mathematics becomes apparent in activities such as manipulation of variables and rote calculations, thus reflecting an algorithmic use of mathematical principles where the mathematics exists independently of any specific physical content. In contrast, structural mathematics actively shapes the underlying form of physical concepts, making it inseparable from its associated physical content (Uhden et al., 2012).

The introduction of this twofold perspective has had significant implications for the discussion on how students' mathematical skills relate to their performance in physics classes, adding nuance to the view of mathematics as a mere prerequisite for learning physics (Karam et al., 2019). While shortcomings in technical skills in mathematics would undoubtedly contribute to students' difficulties in physics courses, this view alone does not provide a complete picture. Proficiency in technical mathematics does not guarantee success in physics, as highlighted by Hudson and McIntire (1977); proficiency in understanding structural mathematics, as integrated in the discipline, is also necessary (Uhden et al., 2012).

Intrigued by the discrepancy found between students' mathematical proficiency and their ability to effectively apply that knowledge when confronted with physics problems, Tuminaro and Redish (2007) conducted a study to investigate how context affects physics students problem-solving strategies. To this end, they adopted *the resources framework* thus considering knowledge as constructed of small cognitive units (resources) that can be activated and connected in different, dynamic, networks depending on the context. Their study showed that students rely on 'limited sets of locally coherent resources', or *epistemic games*, that influence what knowledge and skills that are leveraged in a given problem-solving situation. Tuminaro and Redish (2007) identified six distinct epistemic games, aiming to describe how students engage with mathematics when solving physics problems: mapping meaning to mathematics, mapping mathematics to meaning, physical mechanism game, pictorial analysis, recursive plug-and-chug, and transliteration to mathematics.

The impact of students' epistemological resources on their problem-solving approaches was further explored by Bing and Redish (2009) who proposed the idea of tracing students' *warrants*, i.e. arguments for doing something in a certain way, as a means to capturing students' epistemological framing. *The* *resources framework* is part of the theoretical underpinnings of this work and will be described in more detail in Section 3.1.4.

Students use of mathematics to solve physics problems and make sense of physical phenomena has also been analysed through the lens of *conceptual blending* (also known as *blended processing*): a model of human information integration introduced by Fauconnier and Turner in 1998. According to this model, meaning-making occurs through the selective blending of information from multiple *mental input spaces*, containing knowledge elements that are often activated together (Van den Eynde, 2021). For instance, a learner may have an input space consisting of various mathematical principles, another one containing knowledge of some physics concept, and a third one holding ideas and experiences from everyday life. In order to make sense of an unknown phenomenon, the blended processing model posits the learner to project knowledge from two or more of these input spaces to a *blended space*, which is emergent and specific to the particular learning situation. In other words, the construction of new knowledge takes place in the blended space.

Although the concept of blending was originally introduced by Fauconnier and Turner (1998) its application within PER was pioneered by Bing and Redish (2007) who used *blending diagrams* to visualise students' reasoning. These diagrams illustrate which elements that are blended during a sensemaking or problem-solving activity, along with their corresponding input spaces, thus providing insight into how learners connect and combine ideas from different disciplines. Recently, Van den Eynde (2021) published a thesis on the blending of physics and mathematics, in which she introduced a chronological dimension to the blending process, resulting in the development of *dynamic blending diagrams* (DBDs). Unlike traditional blending diagrams, which typically focus on the outcome of the meaning-making process, DBDs place greater emphasis on the meaning-making process itself.

Unsurprisingly, the interplay between physics and mathematics has also been a focal point of research on undergraduate mathematics education (RUME). Within this field, *the mathematical modelling cycle (MMC)* has gained traction as a promising framework for analysing problem-solving activities that require students to integrate mathematical knowledge with knowledge from other scientific disciplines (Borromeo Ferri, 2006). For example, Jensen et al. (2017) showed that 'unformalised physics problems' presented students with opportunities to engage in mathematisation, which is a modelling step that has been identified as particularly challenging to students.

In my research, I draw inspiration from the extensive body of literature on the teaching and learning of mathematical modelling (Niss & Blum, 2020b), employing the MMC as part of my theoretical framework (Section 3.3.3).

2.2.2 The role of mathematics in chemistry education[I]

The role of mathematics in chemistry education has gained increased attention in recent years. Similar to the discussion within PER, there is an agreement within CER that using mathematics in chemistry is different from doing pure mathematics (Phelps, 2019; Rodriguez et al., 2019a). The majority of research in this area is centred on students' problem-solving strategies in topics that lie at the interface of chemistry and mathematics, such as thermodynamics (reviewed in Bain et al., 2014) and chemical kinetics (reviewed in Bain and Towns, 2016). The relationship between chemistry and mathematics has also been discussed more recently in Towns *et al.*, 2019b.

Given that the primary of focus of this licentiate thesis is on problem solving within the realm of chemical kinetics, the remainder of this section will concentrate on previous research specifically related to the teaching and learning of chemical kinetics. For readers wishing to explore the teaching and learning of thermodynamics in chemistry education, I recommend consulting the comprehensive review by Bain et al. (2014).

Starting in 2018, Bain and colleagues carried out a larger research project exploring university students' understanding and use of mathematics in the context of chemical kinetics. The researchers conducted semi-structured interviews, during which they tasked chemistry students with problems related to zero- and second-order kinetics, prompting them to reason about corresponding mathematical equations and graphs. The data collected underwent analysis through multiple perspectives, including the resources framework, symbolic forms, graphical forms, and blended processing (summarised in Bain et al. 2019).

One study in this project focused on the relationship between students' ability to blend knowledge from different domains and task success (Bain et al., 2018). Analysis revealed two distinct groups: high-frequency blenders, i.e. students who exhibited five or more instances of blending during the interview; and non-blenders, i.e. students who did not blend at all. According to Bain et al. (2018), high-frequency blenders demonstrated expert-like integration of conceptual and mathematical reasoning during the studied problem-solving activities.

In the final phase of this larger project, Rodriguez *et al.* (2020b) examined the influence of students' epistemological resources on their overall problem-solving approaches. Drawing on work by Tuminaro and Redish (2007), Rodriguez and colleagues explored how students transitioned between different epistemic games during a problem-solving activity, concluding that such transitions normally did not occur spontaneously but rather required explicit prompting.

Although showing a positive correlation between task success and high-frequency blending, the combined findings of this series of studies indicate that students generally tend to rely on algorithmic problem-solving strategies, with mathematical reasoning taking precedence over conceptual reasoning even in the presence of blending (Bain et al., 2019).

Students' understanding of various concepts and representations used in enzyme kinetics has also been an area of focus (summarised in Rodriguez & Towns, 2020). More specifically, Rodriguez and colleagues observed second-year undergraduate students as they reasoned about a Michaelis-Menten graph (which describes the relationship between the rate of an enzyme-catalysed reaction and the substrate concentration), and the associated kinetic parameters V_{max} (the maximum reaction velocity) and K_{m} (the Michaelis constant). The data collected from these students were analysed from multiple perspectives.

First, they analysed the data through the lens of the *resources framework,* constructing *resource graphs* (Wittmann, 2006) to visualise how students connected their conceptual understanding of different types of enzyme inhibition to changes in the Michaelis-Menten graph, V_{max} and K_{m} (Rodriguez & Towns, 2019). Next, they analysed the same data through the lens of *graphical forms*, as introduced by Rodriguez et al. (2020), focusing in on students' use of mathematical resources when reasoning about enzyme kinetics, particularly emphasising students' intuitive ideas of certain structural features of a graph (Rodriguez, Bain, & Towns, 2019). Finally, they expanded their analysis to also include students' reasoning about additional representations used in enzyme kinetics, such as Lineweaver-Burk plots and reaction schemes (Rodriguez, Hux, et al., 2019).

The collective findings from these analyses revealed that although students were able to correctly link different kinds of enzyme inhibition with specific changes in the mathematical representations, they often struggled to explain the underlying molecular (or particulate) events driving these changes. (Rodriguez & Towns, 2020).

In another study, Rodriguez *et al.* (2019b) investigated how students approached the analysis of an unfamiliar concentration-and-time graph for a chemical reaction. Drawing on concepts from the resources framework and graphical forms, the researchers focused their analysis on the students' covariational reasoning. The study categorised the variety of productive, unproductive, static and dynamic reasoning that students demonstrated when solving such a task. An open-ended part of the task with no single, definitive answer generated particularly interesting strategies, with some students succeeding in giving a full mathematical narrative for the reaction, showing a high level of integration of chemistry and mathematics.

Taken together, these studies on problem solving in chemical kinetics all indicate that even when students demonstrate proficiency in mathematics, the connection between their mathematical and chemical resources may remain superficial. Thus, students require additional support in creating meaningful connections between their understanding of concepts in chemical kinetics and the mathematical representations used to model those concepts (Rodriguez & Towns, 2020).

2.3 Situating my own research

> Why are we so inept at engaging learners in problem solving? A major reason, I argue, is that we do not understand the breadth of problem-solving activities *well enough* [emphasis added] to engage and support learners in them.
>
> (Jonassen, 2000, p. 63)

As highlighted in the Introduction, there is a gap in our understanding of the challenges faced by students when engaging in problem solving within math-intensive chemistry topics such as chemical kinetics and thermodynamics. I believe that we can address this gap by following the subtle lead provided by Jonassen in the quote above: that is, by obtaining a more profound and detailed understanding of these particular problem-solving activities.

To this end, I combine models and concepts from chemistry, physics, and mathematics education research to develop a framework suitable for analysing the specific hurdles that students encounter when integrating their knowledge in chemistry and mathematics.

In summary, the research presented in this licentiate thesis aligns with the call for interdisciplinary research approaches and investigations into upper-level chemistry courses. Furthermore, my work contributes to advancing our understanding of the challenges related to solving real-world problems, with a special focus on the mathematical modelling of chemical phenomena. By providing a more nuanced characterisation of students' actions during such problem solving, my research adds to the groundwork for developing targeted teaching strategies.

3 Theoretical framework

In this chapter, I present the theoretical framework that undergirds my entire research project. That is, the selected theories, models, and concepts that shape the way I think about my research topic.

The chapter begins with a brief introduction to three **theories of learning** (or learning perspectives): cognitive science, constructivism and sociocultural theory. Subsequently, I describe the resources framework, which is a model of knowledge construction that serves as an analytical framework in my thesis. Following this, I acquaint the reader with theories, models and concepts that relate to **problem solving**. This includes general models of problem solving, the mathematical modelling cycle, procedural knowledge, and metacognition. Additionally, I give an overview of prior research and various definitions of **intuition** – a concept particularly relevant to Paper II and ongoing studies. In the concluding section of this chapter, I highlight the specific assumptions derived from each presented theory, model and concept, that constitute my theoretical framework.

Note that in this work, we have adopted a *subjective inductive approach* with a *theory-informing data analysis*. This means that the theoretical framework was developed alongside the data analysis (Varpio et al., 2020). A more detailed description of this approach is given in Section 5.1.

3.1 Theories of learning

To study *the learning of chemical kinetics*, or the learning of any topic for that matter, it is important to establish how one conceptualises learning. That is, to answer the question: What does it truly mean to *learn* something? Fortunately, many scholars before me have already explored this question, resulting in a plethora of *learning theories*.

A learning theory is a set of principles, or assumptions, that seeks to explain the nature of learning, i.e. how people receive, process, and retain knowledge. For example, *behaviourism* posits that learning occurs through reinforcement of certain observable behaviours, focusing on how learners respond to external stimuli. In contrast, *cognitivism* emphasises the role of mental processes in learning (Schunk, 2020). Each learning theory offers a unique lens through which we can understand how learning occurs.

Note that although the terms ‘learning *theory*’ and ‘learning *perspective*’ are sometimes used interchangeably, they are not the same. Strictly speaking, a learning *perspective* is a much broader term. It concerns a way of viewing the process of learning (rather than a set of specific principles as is the case of a learning *theory*) and may, in fact, encompass multiple learning *theories*.

In this thesis, I predominantly rely on *cognitive science* (a learning theory) and *constructivism* (a learning perspective). For future work, I might also draw from *sociocultural constructivism* (a certain branch of constructivism).

3.1.1 Cognitive science

Before diving into any details, I would like to clarify that cognitive science is a scientific theory that captures many more aspects of cognition than learning alone: drawing from a multitude of fields (e.g. linguistics, psychology, neuroscience, philosophy, computer science and anthropology), cognitive science seeks to understand the nature, the tasks, and the functions of cognition (Miller, 2003). However, for the purpose of this thesis, whenever I refer to cognitive science, I specifically mean *cognitive science as a learning theory*.

As a learning theory, cognitive science emphasises the role of learners’ mental processes in shaping both their behaviour and understanding. Unlike some behaviourist theories, which focus solely on observable actions, cognitive science seeks to explore the internal cognitive structures and mechanisms that drive these actions. A key tenet of cognitive science is therefore the assertion that it is possible to gain insights into an individual’s mind by examining their actions and the manner in which they execute them (Schunk, 2020).

In education, cognitive science promotes instructional strategies that align with how the mind processes information, highlighting the importance of active engagement, meaningful connections, and the use of various cognitive strategies to enhance learning outcomes. By gaining insights into the cognitive mechanisms at play, educators can design learning experiences that optimise the way students acquire and retain knowledge (Schunk, 2020).

3.1.2 Constructivism

Constructivism is a learning perspective which posits that learners *construct* their own knowledge and understanding of the world, and that they do so by building upon their prior experiences. Thus, a key assumption of constructivism is that learners are *active* participants in their own learning journey. Rooted in the epistemology that individuals must actively construct their own knowledge, and that knowledge cannot be passively acquired, constructivist theorists reject the idea of fixed scientific truths awaiting discovery; instead, they view knowledge as a working hypothesis (Schunk, 2020).

As mentioned earlier, a learning perspective may encompass multiple theories. Such is the case of constructivism, which is essentially a family of theories that vary in how they view the process of construction (Schunk, 2020): from those that postulate complete self-construction (e.g. Piaget and Bruner) to those that hypothesise socially mediated construction (e.g. Vygotsky, see Section 3.1.3).

In education, constructivism suggests that we structure teaching and learning experiences to challenge students' thinking, enabling them to construct new knowledge. Instructional approaches such as problem-based learning and inquiry-based learning align with the principles of constructivism, providing opportunities for learners to actively engage, reflect on their thinking process, and collaborate with peers (Schunk, 2020).

The essence of constructivism lies in the idea that learners build on their previous experiences when acquiring new knowledge.

3.1.3 Sociocultural theory

The sociocultural branch of constructivism, also referred to as *sociocultural theory*, was introduced by Vygotsky (1978). It acknowledges and emphasises the influence of social and cultural contexts on learning. Essentially, sociocultural theorists view learning a collaborative endeavour, where knowledge is co-constructed through shared experiences and interactions among individuals within their social environment.

According to sociocultural theory, language plays a pivotal role, enabling learners to articulate their thoughts both to others and to themselves. Vygotsky distinguishes between three types of speech, stating that learners engage in: *social speech* while discussing out loud with peers; *private speech* while vocalising thoughts aloud to themselves; and *inner speech* when expressing thoughts 'mentally' without vocalising them (Schunk, 2020).

An important concept within sociocultural theory is the 'zone of proximal development' (ZPD), representing the difference between what learners can achieve independently and what they can attain with assistance from others. According to sociocultural theory, interactions with adults and peers within the ZPD promote cognitive development (Schunk, 2020).

In education, sociocultural theory advocates for collaborative and interactive learning experiences, promoting the creation of supportive social environments where learners can engage in meaningful interactions, share perspectives, and co-construct knowledge. The role of the educator in this theory is that of a facilitator who guides and scaffolds learners within their ZPD, fostering a dynamic and socially mediated learning process (Schunk, 2020).

3.1.4 The resources framework[I]

The resources framework is an analytical framework that draws from cognitive theory, constructivism, neuroscience and information processing theory. Building on ideas put forth by several prominent scholars within the field of PER (e.g. Clement et al., 1989; diSessa, 1993; Hammer, 2000; E. Redish, 2004), it proposes that knowledge is constructed from fine-grained cognitive units known as *resources*, which are connected to each other in dynamic networks (Hammer et al., 2005).

There are three main types of resources: conceptual, procedural, and epistemological. Conceptual resources pertain to knowledge of specific concepts, e.g. understanding the relationship between kinetic energy and the state of matter. Procedural resources encompass practical knowledge or 'know-how', e.g. knowing how to apply the ideal gas law to estimate the volume of a gas. Epistemological resources relate to a learner's perspective on what counts as knowledge, e.g. considering a piece of information valid because 'the teacher said so' or because 'I made it up' (Hammer & Elby, 2002, 2003).

It is important to understand that these resources are smaller in size than concepts or abilities as experienced by learners. In other words, the concept of a ball or the ability to kick a ball, consist of multiple resources rather than being standalone resources themselves (Hammer et al., 2005).

The neuroscientific view is reflected in the framework's emphasis on resources being connected in networks that are *dynamic* and *emergent*, rather than static structures. This aligns with the current understanding of the human brain as a collection of neurons that connect to each other in dynamic networks to execute various physical and cognitive functions.

Viewing knowledge through this lens has interesting implications for several learning principles, including transfer. Instead of treating learned concepts and abilities as fixed entities that are either transferred or not, researchers within the resources tradition consider learners to possess various resources that can be *activated* and employed differently depending on the context (Hammer et al., 2005). This perspective enables us to understand how the same student may exhibit different, at times contradictory, reasoning and problem-solving approaches in response to certain settings. As such, the resource framework attempts to account for more momentary activation of different cognitive structures in different contexts, rather than considering robust and more fixed conceptions.

The context is said to play a crucial role in *framing* problem-solving activities, influencing how learners respond to questions like 'What is going on here?' and 'What is this about?'. Essentially, framing can be understood as the learner's perception or interpretation of a given situation, which in turn affects what network of resources is activated. For example, if a student frames a task as being about history, this is likely to trigger the activation of other resources than if the student perceives the task as being about biology.

Researchers within the resources tradition typically do not consider resources as being right or wrong; rather, they view the *activation* of certain resources as productive or unproductive in a given context (Hammer et al., 2005).

Within PER, the resources framework has been applied to explore problem-solving approaches and conceptual change among physics students (Hammer & Elby, 2003; Richards et al., 2020; Wittmann, 2006; Wittmann et al., 2019).

In recent years, the framework has also made its way into CER, particularly in studies investigating the interplay between mathematical and chemical resources (Rodriguez, Bain, & Towns, 2019; Rodriguez, Bain, Towns, et al., 2019).

3.2 Problem solving

> There are only two critical attributes of a problem. First, a problem is an unknown entity in some situation (the difference between a goal state and a current state) … Second, finding or solving for the unknown must have some social, cultural, or intellectual value. That is, someone believes that it is worth finding the unknown. If no one perceives an unknown or a need to determine an unknown, there is no perceived problem (…). *Finding the unknown is the process of problem solving* [emphasis added].
>
> (Jonassen, 2000, p. 65)

The aim of this section is to introduce the reader to prior research related to the teaching and learning of problem solving. I have chosen to keep this review rather condensed, with a primary focus on analytical frameworks and concepts relevant to my research.

To discuss problem solving, we must first address the question of *what constitutes a problem* and *how to define problem solving*.

The answer to the first question is well captured by Jonassen (2000), who describes a problem as ‘an unknown entity,’ further specifying that it is ‘the difference between a goal state and a current state.’ As a complement this definition, I underscore that a problem is never solely defined by its content but also depends on the problem solver; what poses a challenge to one learner may not necessarily present a difficulty for another.

So, what is problem solving, then? Again, drawing from Jonassen (2000), it is the process of ‘finding the unknown’. A more informative definition is that problem solving is *a sequence of cognitive operations that involve identifying, analysing, and developing strategies to overcome a challenge* (Jonassen, 2000; Schunk, 2020).

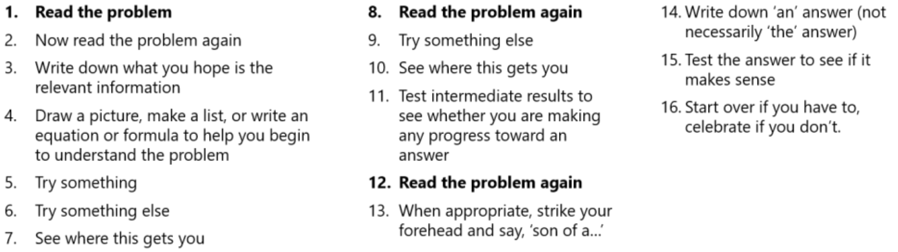
The significance of problem-solving skills is apparent not only in research literature (Gagné, 1985; Jonassen, 2000; Tsaparlis, 2021) but also in various reports from global institutions such as the United Nations and the World Economic Forum, which recognise problem-solving skills as paramount for the workforce of the future (Elkeiy, 2022; United nations, 2023; World Economic Forum, 2020). Furthermore, people worldwide need problem-solving skills in several aspects of life, from navigating personal dilemmas to resolving work-related tasks. Problem-solving skills are undoubtedly important. The question is, how do we promote the development of these skills? And in an educational setting, how should we teach them effectively?

In tackling these questions, a first step is to gain a better understanding of the cognitive mechanisms that underlie problem solving. Several models have been proposed, and while I will not provide an exhaustive review, I will draw inspiration from Bodner (2003) and compare two rather different models: *Polya's four stages model* and *Wheatly's anarchistic model*.

3.2.1 Models of problem solving

In 1945, Polya proposed the following four steps as a model of problem solving: Step 1 – understand the problem, Step 2 – devise a plan, Step 3 – carry out the plan, and Step 4 – look back. While this model may seem logical at first glance, there is no empirical evidence supporting it; researchers have not been able to demonstrate that these are the steps followed by either experts or novices during problem solving (Bodner, 2003).

About 40 years later, Wheatley proposed another set of steps to model the art of problem solving (Wheatley, 1984). Although Wheatley's anarchistic model (Figure 2) was likely formulated with a glint in his eyes, it does prove a point: problem solving is an *iterative* process.



1. **Read the problem**
2. Now read the problem again
3. Write down what you hope is the relevant information
4. Draw a picture, make a list, or write an equation or formula to help you begin to understand the problem
5. Try something
6. Try something else
7. See where this gets you
8. **Read the problem again**
9. Try something else
10. See where this gets you
11. Test intermediate results to see whether you are making any progress toward an answer
12. **Read the problem again**
13. When appropriate, strike your forehead and say, 'son of a...'
14. Write down 'an' answer (not necessarily 'the' answer)
15. Test the answer to see if it makes sense
16. Start over if you have to, celebrate if you don't.

Figure 2. Wheatley's anarchistic model of problem solving.

I want to clarify here that I am not suggesting that Polya's model is wrong or inferior to Wheatley's. Rather, I wish for this comparison to illustrate that these models represent different archetypes: Polya's model is idealised, reflecting a goal state rather than the reality. It is a *prescriptive* model, offering guidelines for essential steps that an ideal problem-solving process *should* include. In contrast, Wheatly's model is more realistic, reflecting the actual sequence of steps that problem solvers engage in; it is *descriptive* in its nature.

The advantage of an idealised model lies in its simplicity and ease of use. However, a model's utility must always be assessed in relation to its intended purpose. If we aim to help students improve their problem-solving skills, we need insight into what students actually do during problem solving. Thus, adopting a more realistic model might be more beneficial. On the other hand, attempting to apply a ‘messy’ model such as Wheatly’s may introduce practical difficulties in the data analysis process. For this purpose, opting for a simpler model could prove more effective. All this to underscore the point that when selecting a model to describe a particular phenomenon, there is always a trade-off between simplicity and accuracy that one must carefully consider.

In this thesis, I discuss findings from two studies exploring a specific kind of problem solving: that which occurs at the interface of chemistry and mathematics. For this purpose, I employ *the mathematical modelling cycle* (MMC; Borromeo Ferri, 2006). The MMC is an idealised model describing the most essential steps in mathematical modelling of real-world problems (Czocher, 2014). In Paper I, I build on the classical MMC, developing a more descriptive version that better captures the actual steps that students engage in during problem solving at the interface of chemistry and mathematics (the *extended* MMC; Ye et al., 2024). The MMC is part of my theoretical framework and is described in more detail in Section 3.3.3.

3.2.2 Problem solving in CER

A considerable amount of the CER literature on problem solving revolves around mapping students’ difficulties with open- and closed-end problems, with findings consistently indicate that students exhibit greater proficiency in solving closed-end problems (Cooper & Stowe, 2018). This resonates with conclusions drawn from studies on problem solving in math-heavy topics, as outlined in Section 2.2.2: although students may demonstrate competence in performing calculations, they frequently struggle in attributing meaning to their calculations.

Another focus of CER in this area has focused on students’ approaches to problem solving specifically in organic chemistry. Readers interested in this domain are advised to explore the following review articles: *The Tip of the Iceberg in Organic Chemistry Classes: How Do Students Deal with the Invisible?* – a review of problem-solving behaviour in organic chemistry by Graulich (2015); and the more review by Dood and Watts (2023) titled *Students’ Strategies, Struggles, and Successes with Mechanism Problem Solving in Organic Chemistry: A Scoping Review of the Research Literature*.

Within CER, the examination of problem solving has predominantly been approached through the lens of information processing theory. A posited by Johnstone and his chemistry triplet (Johnstone, 1991), ideas from cognitive load theory can explain students’ struggles in making sense of chemical concepts and solving problems in chemistry: the cognitive load of a task is inversely correlated with task success and the multi-level thinking required by chemistry inevitably places a high cognitive load on learners.

3.2.3 What makes a successful problem solver?

According to Mayer (1998), there are three key components that distinguish a successful problem solver from an unsuccessful one: skill, metaskill and will. *Skill* corresponds to domain-specific knowledge, encompassing the problem solver's proficiency in applying relevant information and techniques to a given task. *Metaskill* or *metacognition* involves the ability to control and monitor cognitive processes. It goes beyond the mastery of skills, emphasising the problem solver's capacity to regulate their thinking, strategically deploy resources, and adapt their approach based on the demands of the task at hand. Essentially, metacognition serves as an orchestrator, coordinating the various cognitive resources and processes involved in effective problem solving. *Will* relates to the impact of motivation on cognition. It concerns the problem solver's feelings and interest in solving a task, asserting that meaningful contexts and personal investment enhance problem-solving skills. Will is sometimes referred to as *grit* and underscores the intrinsic motivation, passion, and perseverance required to tackle nonroutine problems successfully.

While I recognise the importance of will (or grit) in problem solving, the exploration of this component is currently outside the scope of this thesis. Rather, the focus of my thesis is on the cognitive and metacognitive aspects of problem solving. In the following sections, I will explore some key concepts related to problem solving that are relevant for the discussion in this thesis. This includes *procedural knowledge* and *metacognition.*

3.2.4 Procedural knowledge[II]

Procedural knowledge pertains to the knowing of how to perform a specific task or skill and is sometimes referred to as 'know-how'. This type of knowledge extends beyond verbal articulation, meaning that an individual may possess procedural knowledge without necessarily being able to express it in words: as long as they can execute the steps and techniques required to successfully carry out a particular activity, they possess procedural knowledge of that activity (McCormick, 1997).

In this thesis, I have adopted a terminology proposed by Star (2005) which distinguishes between *deep* and *superficial* procedural knowledge. In 2005, Star scrutinised the definition of procedural knowledge, challenging the then prevailing perception of it as mainly algorithmic and, consequently, less coherent and comprehensive than conceptual knowledge. Star attributed the negative connotation associated with procedural knowledge to a conflation between knowledge *type* and knowledge *quality* embedded in the definitions of conceptual and procedural knowledge introduced by Hiebert and Lefevre in the mid-80s.

Hiebert and Lefevre (1986) defined conceptual knowledge not just as knowledge of concepts and principles (type) but also included a dimension of 'richness', stating that conceptual knowledge 'can be thought of as a connected web of knowledge, a network, in which the linking relationships are as prominent as the discrete pieces of information'. Similarly, procedural knowledge was described not only as knowledge of procedures (type) but also as being more sequential, and thus superficial, in comparison to conceptual knowledge.

Star (2005) emphasised that richness and superficiality pertain to the *quality* of knowledge rather than its *type*. In an effort to disentangle these two dimensions, he proposed a reconceptualisation, keeping the traditional definitions of knowledge *type*, i.e. viewing conceptual knowledge as 'knowledge of concepts' and procedural knowledge as 'knowledge of procedures', while introducing also a dimension of quality to both types of knowledge, thus allowing for conceptual as well as procedural knowledge to exist on a spectrum ranging from deep to superficial. An important outcome of this reconceptualisation is that procedural knowledge can be considered deep without necessarily being tied to conceptual knowledge; it can stand on its own.

According to Star (2007), students with deep procedural knowledge are flexible in how they apply procedures, apply procedures with critical judgment, and can explain *how* to apply a certain procedure in order to achieve a certain goal. Note that Star's reconceptualisation does not imply that procedural and conceptual knowledge must always be seen as separate; on the contrary, Star acknowledges that conceptual knowledge can contribute to the depth of procedural knowledge. His point is that procedural knowledge can also be deep on its own.

3.2.5 Metacognition[II]

> 'Metacognition' refers to one's knowledge concerning one's own cognitive processes and products or anything related to them. (…) Metacognition refers, among other things, to the active monitoring and consequent regulation and orchestration of these processes in relation to the cognitive objects on which they bear, usually in the service of some concrete goal or objective.
>
> Flavell, 1976, p. 232

While the *concept* of metacognition had been explored by various researchers before him, the introduction and popularisation of the *term* metacognition are frequently attributed to Flavell (1976). As elucidated by the quote above, metacognition can be divided into two key facets[2]: metacognitive knowledge and metacognitive regulation.

Metacognitive knowledge includes the conscious awareness of one's own cognitive processes and the factors that influence them. This category can be further divided into three subclasses: declarative, procedural and conditional knowledge. In some contexts, declarative knowledge is equated with factual information, such as 'Stockholm is the capital of Sweden.' However, in the context of metacognition, declarative knowledge typically refers to what you know about yourself as a learner; for instance, what factors that may influence your capacity to learn. Procedural knowledge revolves around strategies, e.g. knowing that certain parts of a scientific paper can be skimmed while others should be read more thoroughly. The third subclass, conditional knowledge, refers to the understanding of when and why to apply a particular strategy (Schraw et al., 2006). *Metacognitive regulation* entails the active control of cognitive processes; it involves planning, monitoring, and evaluating one's thinking (Flavell, 1979).

Metacognitive competence has been identified as a potential means to foster students' conditional knowledge. That is, their knowledge of *when* to apply various strategies, such as intuitive or analytical reasoning, during problem-solving activities. Given that the focus of this thesis is on problem solving that involves mathematical modelling of chemical phenomena, I will now introduce two analytical frameworks, proposed in the field of RUME, that focus on metacognitive actions during mathematical problem solving. One of these is known as *the cognitive-metacognitive framework* (Garofalo & Lester, 1985) and the other is a map illustrating various metacognitive pathways that may lead to failure (Goos, 1998, 2002). To my knowledge, the latter does not go by any specific name; I will refer to it as *Goos's metacognitive pathways*.

3.2.5.1 The cognitive-metacognitive framework

Building on previous work by several scholars in RUME (Luria, 1973; Polya, 1945; Schoenfeld, 1992; Sternberg, 1980, 1982), Garofalo and Lester (1985) developed a framework intended to serve as a tool for researchers interested in analysing the metacognitive aspects of mathematical performance. Their *cognitive-metacognitive framework* consists of four main categories, representing the different phases of solving a task in mathematics: *orientation* (strategic behaviour to assess and understand a problem); *organisation* (planning of behaviour and choice of actions); *execution* (regulation of behaviour to conform to plans); and *verification* (evaluation of decisions made and of outcomes of executed plans). Garofalo and Lester (1985) further divide each main phase into subphases, some of which correspond to metacognitive behaviours such

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[2] In some literature on metacognition, a third component called *metacognitive experience* is mentioned. Metacognitive experience concerns the feelings evoked during problem solving (Flavell, 1979). This component is outside the scope of this thesis.

as planning what to do, monitoring while doing, and evaluating what has been done.

3.2.5.2 Goos's metacognitive pathways

In 1998, Goos highlighted a deficiency among the analytical frameworks used for investigating mathematical problem solving at the time: while most of these frameworks acknowledged the central role of metacognitive actions, they lacked the necessary detail to effectively guide such actions. More specifically, Goos (1998, 2002) meant that they did not provide enough detail on various *types* of monitoring and regulatory activities, and stressed the importance of distinguishing between *routine monitoring*, i.e. checking that 'all is well', and *controlled regulatory responses* that typically arise when students find themselves in 'moments of uncertainty'. To address this issue, Goos introduced the concept of metacognitive 'red flags' as a way to identify events or objects that *trigger* metacognitive actions, enabling a more precise recognition of when regulatory activities are initiated.

Three types of red flags were proposed: lack of progress, error detection, and anomalous results. Metacognitive *success* is achieved when problem solvers recognise a red flag and take appropriate measures to deal with the difficulty, or recognise that nothing is wrong, leading them to continue on the same solution path. However, engaging in metacognitive actions does not guarantee task success. A significant contribution from Goos's research is the introduction of different kinds of metacognitive *failure*: blindness, vandalism, and mirage. The diagram in Figure 3 (adapted from Goos, 2002) illustrates how these categories relate to the path, or trajectory, of a problem-solving attempt. Metacognitive blindness occurs when a problem solver fails to recognise a red flag even though it is present. The opposite case is referred to as metacognitive mirage: when a problem solver believes there is a red flag (i.e. that something is wrong) although there is not. The final category, metacognitive vandalism, describes situations where the problem solver has identified that some kind of response is needed but executes an inappropriate one. An example of this is when students, instead of changing their own problem-solving strategy, alter their interpretation of the problem to fit their original strategy.

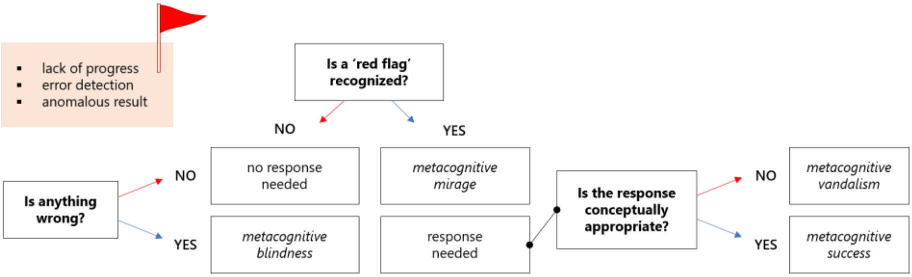

Figure 3. Goos's metacognitive pathways, redrawn from Goos (2002).

3.3 Mathematical modelling

All models are wrong, but some are useful.

(Box, 1979, p. 202)

Before delving into a discussion of mathematical modelling, it is wise to first establish the concept of a model. Simply put, a *model* is a representation of something else (Niss & Blum, 2020b). Expanding on this minimalist definition, George Box's famous (and also rather minimalistic) saying captures the essence of models as *simplified* representations, meaning that they capture only selected features of the objects or phenomena they represent. A *mathematical model,* then, can be described as a certain kind of model that represents extra-mathematical phenomena in terms of mathematical symbols and relationships. The term *extra-mathematical* is used to describe all that which resides beyond the realm of pure mathematics.

This brings us to the act of *mathematical modelling*, which corresponds to the bidirectional process of translating between the real-world domain and the mathematical domain (Blum & Borromeo Ferri, 2009).

The significance of mathematical modelling thus lies in its role of bridging mathematics with the real world, and the ability to engage in mathematical modelling is globally recognised as a fundamental goal of mathematics education. Furthermore, while mathematical modelling is a crucial skill in itself, it has also been shown to promote the development of other essential problem-solving skills. In other words, it operates both as an objective and a strategy for learning.

The following sections begin with an overview of the historical development of mathematical modelling in education (Section 3.3.1). Subsequently, I offer a brief account of the current state of the field, i.e. *what we know* about mathematical modelling in education (Section 3.3.2). Finally, I introduce the reader to the mathematical modelling cycle, which is a crucial part of my theoretical framework (Section 3.3.3.).

3.3.1 The historical development of research on mathematical modelling in education

The history of mathematical modelling in education dates back to the 1970s. In contrast to CER, where there is a lack of research in upper-level courses, much of the early efforts in mathematical modelling education research took place at the university level. This inclination was likely due to the perception of the topic as too complex for pre-college education.

Similar to the historical development of CER, research on the teaching and learning of mathematical modelling can be divided into two distinct periods. Before delving into each wave, I would like to highlight that in its early stages, the field of mathematical modelling education research was concerned with both mathematical modelling *and its application*. While modelling refers to the complete process of translating back and forth between the real-world and the mathematical domain, application entails merely the utilisation of a model.

During the first wave (1970-1995), the primary concern of the field was essentially to establish itself in the broader realm of mathematics education research. This led to an emphasis on three main objectives: (A1) advocating for the inclusion of mathematical modelling and application in mathematics curricula at all educational levels, providing evidence for practical realisation, and establishing a common terminology within the field; (A2) shedding light on successful implementations of mathematical modelling in curricula to demonstrate the viability of these ideas in real-life situations; and (A3) disseminating examples of modelling and application suitable for educational materials, making them accessible to teachers (Niss & Blum, 2020b).

In the second wave (1995-today), the field underwent three major changes: (B1) a reduced emphasis on applications; (B2) a heightened focus on students' difficulties in grappling with mathematical modelling, placing emphasis on the processes and sub-processes of modelling and the notion of modelling competencies; and (B3) received recognition as a legitimate research strand within the field of mathematics education research (MER).

Today, the field of mathematical modelling education research has evolved into a strong community of researchers and practitioners referring to themselves as *The International Community of Mathematical Modelling and Applications (ICTMA).* Since 1983, the community hosts a biennial conference on the teaching and learning of mathematical modelling (Niss & Blum, 2020b).

3.3.2 The current state of research on mathematical modelling in education

The research literature on mathematical modelling in education is extensive, covering a wide range of topics. For readers eager to delve into this field, I recommend exploring the book series titled *International Perspectives on the Teaching and Learning of Mathematical Modelling*, which effectively captures the ongoing developments in the field.

In a relatively recent book published by Niss and Blum (2020b), they present an overview of 'evidence from empirical research' on the teaching and learning of mathematical modelling. I summarise these insights below, presenting eight key aspects that *we know* about mathematical modelling in education.

1 – Learning and cognition is situated. Research suggests that learning is situated, implying that knowledge acquired in one context is typically linked to certain indices of that setting and thus, may not easily transfer to another

(Watson, 1998). For example, students who have learned about differential equations in a purely mathematical setting, such as a maths course, cannot be expected to automatically apply that knowledge in a chemistry course.

On a more positive note, there is evidence that we can increase the chances of transfer through explicit instruction (Anderson et al., 1996). By making students aware of and conscious about the distinct steps of the modelling process, we can increase the chances of successful transfer.

Altogether, these findings suggest that we cannot expect transfer to occur without explicit support.

2 – Successful mathematical requires certain modelling competencies and sub-competencies. The term *mathematical modelling competency* refers to the ability to 'autonomously and insightfully carry through all aspects of mathematical modelling in a certain context (Blomhoj & Jensen, 2003, p. 126). Essentially, this means that proficient modellers possess two main abilities: (1) the ability to *construct* mathematical models in diverse domains, contexts and situations, i.e. to use mathematics to describe and analyse extra-mathematical phenomena; and (2) the ability *analyse* and critically examine already existing mathematical models in terms of their foundation, their scope and their validity. That is, to judge the appropriateness of a model in relation to a given context, thus aligning with the insightful perspective articulated by Box (p. 52) that 'all models are wrong, but some are useful.'

The first aspect of mathematical modelling competency, i.e. to be able to construct a model, can be broken down into several *sub-competencies*. These typically include pre-mathematisation, mathematisation, mathematical work, interpretation and validation. Unpacking modelling competency in this manner is serves the dual purpose of facilitating the teaching as well as the learning of mathematical modelling.

It is worth noting that there are various ways to 'cut the cake,' meaning that which processes that are considered sub-competencies may vary among publications (e.g. Kaiser & Brand, 2015; Niss & Blum, 2020a). However, regardless of how the cut is made, these sub-processes often align with the steps outlined in a corresponding modelling cycle. A frequently cited modelling cycle will be further discussed in Section 3.3.3.

3 – Mathematical modelling is a challenging endeavour. While mathematical modelling is generally difficult for students, certain steps have emerged as particularly challenging.

In the Danish context, the matter has been thoroughly investigated by Niss and colleagues (e.g. Jankvist & Niss, 2020; Jensen et al., 2017; Niss, 2017) with their findings collectively pointing to pre-mathematisation and mathematisation as significant hurdles. Similarly, Frejd and Ärlebäck (2011) found that Swedish upper secondary students struggled primarily to formulate simplifying assumptions about real-world situations. Note that the simplification step is considered part of the pre-mathematisation process.

Another intriguing observation in this area is the presence of what may be considered a sort of ‘null step barrier’. That is, the mere agreement of a student to undertake a task at all. This insight emerged from a Danish study where it was noted that many students did not view modelling as ‘real maths’ and consequently did not engage seriously with modelling tasks (Jankvist & Niss, 2020).

4 – Successful pre-mathematisation and mathematisation requires the ability to anticipate forthcoming moves. Niss (2010) has proposed the lack of *implemented anticipation* as a possible explanation for students’ difficulties with pre-mathematisation and mathematisation.

Implemented anticipation involves to the ability ‘to *anticipate* (…) forthcoming moves in the modelling process’ (Jankvist & Niss, 2020, p. 470) and ‘to *implement* this anticipation in terms of decision and actions that frame the next step to be made’ (Niss, 2010, p. 56); think of it as having a ‘Spidey sense’ in mathematical modelling.

Both during pre-mathematisation and mathematisation, implemented anticipation requires the modeller to project oneself into a situation that does not yet exist. During pre-mathematisation, the modeller must imagine which elements, and which relationships between elements, from the real-world situation that could be subjected to mathematisation. During mathematisation, the modeller has to implement anticipation in two directions: considering which mathematical terms and relationships that may accurately represent the selected elements of the real-world situation, and simultaneously evaluating whether these mathematical relationships will lend themselves to productive mathematical work and thereby provide mathematical results (Niss, 2010).

Evidently, implemented anticipation is a challenging endeavour; it is not difficult to imagine that this might place a significant demand on learners’ cognitive capacity.

5 – Mathematical modelling routes are individual. Contrary to what is conveyed by most modelling cycles, i.e. that modelling occurs in a linear step-by-step fashion, research shows that modellers exhibit unique and rather irregular modelling routes (Borromeo Ferri, 2006; Doerr et al., 2017). This presents challenges for both researchers and practitioners. In research, analysing learners’ modelling behaviours may become more intricate. In the classroom, the non-linear nature of mathematical modelling makes it less amenable to well-structured teaching strategies, such as following a protocol; the open-ended nature of modelling problems places greater demands on the efforts of students and teachers alike.

6 – Effective teaching strategies for mathematical modelling competency should involve active learning, promote metacognition and present students with diverse opportunities to discover modelling on their own. Research has shown that instructors seeking to deliver high-quality teaching of mathematical modelling should structure their classes in a manner such that there is time for students to discover modelling *on their own*. This approach aligns with the principles of POGIL (Section 2.1.1.6), emphasising the crucial role of students *actively* engaging in their own learning.

Importantly, this activation should encompass both cognitive and metacognitive processes: students should be encouraged to reflect not only on the modelling processes (cognitive activation) but also on the process of modelling itself (metacognitive activation). Evidence suggests that such reflection is essential for students to develop their own knowledge structures of modelling, thus aligning with a cognitive constructivist view of learning.

In addition, to mitigate the ‘issue’ of situated learning, students should be presented with opportunities to tackle mathematical modelling tasks spanning various levels of difficulty and extra-mathematical contexts (Ärlebäck & Doerr, 2015).

These pedagogical strategies collectively contribute to creating learning environments that may foster the development of modelling competency.

As a final note, it is worth recognising that the teaching strategies for mathematical modelling are sometimes categorised into an *atomistic* and a *holistic* approach. An atomistic approach places emphasis on the development of individual modelling sub-competencies, breaking down the intricacies of mathematical modelling into manageable components. Conversely, a holistic approach focuses on modelling competency as a cohesive whole, emphasising the interconnected nature of various sub-competencies. These distinct approaches each have their strengths and limitations. While the atomistic approach allows for a detailed examination and targeted development of specific skills, the holistic approach offers a comprehensive understanding of mathematical modelling as an integrated process. Recognising the merits of both, a mixed approach is typically advised (Kaiser & Brand, 2015; Niss & Blum, 2020b).

7 – Mathematical modelling competency is difficult to assess in a direct manner. When designing assessment instruments for mathematical modelling competency, it is crucial to balance practical ease of conducting and grading with the integrity of used modelling tasks employed, ensuring they maintain their essence and are not oversimplified (Niss & Blum, 2020b).

Historically, written reports have been popular for gaining insight into students’ modelling competencies. A disadvantage of such tests is that they are *indirect*, reflecting only the final outcome of the cognitive processes involved in the modelling procedure. In order to also delve into the internal cognitive processes, methods like interviews and/or observations are necessary.

Today, there exist numerous guidelines for the assessment of mathematical competency, often corresponding to a modelling cycle and adopting either a holistic or an atomistic approach. In a review by Frejd (2013), five common assessment types were identified: written tests, projects, hands-on tests, portfolios, and contests. The choice of assessment type and approach depends, of course, on the purpose of the assessment.

8 – Mathematical modelling activities can serve as vehicles for learning mathematics. There is compelling evidence suggesting that mathematical modelling not only enhance the understanding of various mathematical concepts but also foster the development of general problem-solving skills. Thus, while mathematical modelling should, in itself, stand as a fundamental learning objective in mathematics education, it can also serve as a valuable pedagogical tool for exploring other mathematical topics (Niss & Blum, 2020b).

Having outlined the history and the current state of research on mathematical modelling in education, I will now introduce *the mathematical modelling cycle* – a frequently employed framework for analysing mathematical modelling.

3.3.3 The mathematical modelling cycle[I]

The mathematical modelling cycle (MMC), introduced by Borromeo Ferri (2006), aims to elucidate the fundamental steps (or sub-competencies) involved in mathematical modelling of real-world situations. Various versions of the MMC have been proposed (Niss & Blum, 2020b; Uhden et al., 2012), with a frequently cited version being that by Borromeo Ferri (2006; Figure 4). In the description that follows, all processes (sub-competencies) are written in italics for clarity.

After *understanding* the real situation, the modeller constructs a mental model, *simplifies* the mental model into a real model by determining which parameters that are relevant for the context of the problem, and carry out *mathematisation* of the real model into a mathematical model by translating the chosen parameters into mathematical relationships. Once a mathematical model has been established, the modeller can perform *mathematical work* (i.e. calculations and mathematical manipulations) to obtain a mathematical result.

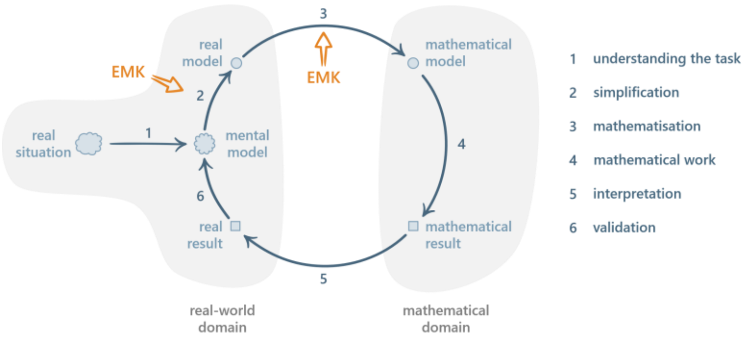

Figure 4. Mathematical modelling cycle, redrawn from Borromeo Ferri (2006); EMK: extra-mathematical knowledge.

To close the cycle, the mathematical result has to be *interpreted* into a real result, which in turn can be *validated* against the real model.

As previously mentioned, there is evidence that mathematical modelling is generally difficult for students, with pre-mathematisation (which includes constructing and simplifying) and mathematisation standing out as particularly challenging steps (Jankvist & Niss, 2020). Borromeo Ferri (2006) has proposed the steps *simplifying/structuring* and *mathematising* to require input from extra-mathematical knowledge (EMK; orange arrows in Figure 4). Since EMK is defined as knowledge other than mathematical such, these steps serve as particularly interesting focal points for the investigation of how students' knowledge in different disciplines interact during problem solving. Note that Ho *et al.* (2019) has in addition pointed out that input from EMK is necessary even in the interpretation and validation phases, especially where mathematical results consist of symbolic and/or complex mathematical expressions.

In the context of CER, the MMC has been employed in a number of studies investigating German high school (Goldhausen & Di Fuccia, 2021; Schmidt & Di Fuccia, 2014) and university students' Komor et al. (2021) engagement in mathematical modelling of chemical phenomena. Additionally, Ho et al. (2019) has discussed and proposed the potential of this framework for analysing the processes at play when students engage in problem-solving activities in chemical kinetics.

As a final note, it is crucial to recognise that the MMC as illustrated in Figure 4 is an idealised model – a point that has been emphasised in the relevant mathematics education research literature (e.g. Blum and Borromeo Ferri, 2009; Prediger, 2009; Doerr et al., 2017). While it serves as a useful representation of the fundamental steps involved in mathematical modelling of real-world problems, it does not take into account the individual differences of students engaging in said activity. Instead, people tend to 'bounce around' (Doerr et al., 2017) different parts of the cycle in a non-linear manner.

3.4 Intuition[II]

What is intuition? The Oxford English Dictionary defines the use of the term in modern philosophy as 'The immediate apprehension of an object by the mind without the intervention of any reasoning process; a particular act of such apprehension.' The word itself stems from the Latin word *intueri* meaning 'to look at, consider' and the late middle English word *intuition* meaning 'insight, immediate cognition, spiritual perception'. In other words, intuition describes a sense of 'just knowing' without being able to fully explain the origins of the knowing. Ironically, this rather elusive characteristic also mirrors the very essence of intuition: we all use it and recognise it, but when asked about what it is and where it comes from, we often stumble, simply attributing it to a ‘gut feeling’.

The somewhat mystical air of intuition has long intrigued scholars across various fields, particularly in philosophy and psychology, resulting in a range of theories and models attempting to describe the phenomenon. The purpose of this section is to provide the reader with a comprehensive introduction and overview of the extensive literature on intuition, offering a general perspective before delving into more specific discussions about intuition in the context of problem solving within the natural sciences.

The concept of intuition is closely intertwined with that of expertise, making it virtually impossible to explore one without also addressing the other. The different perspectives on the interplay between intuition and expertise can be thought of as a spectrum.

At one end of the spectrum, there are those who regard intuition as equivalent to expertise, as proposed by Dreyfus and Dreyfus (1986) and their *five-stage theory of expertise*. According to this theory, intuition is the immediate manifestation of an expert’s holistic understanding of a given situation. This sentiment is reflected in their assertion that ‘experts don’t solve problems and don’t make decisions; they do what normally works.’ That is, intuitive actions are seen as the actions of experts; deliberation, analytical thinking and rule-following are characteristics that typify non-experts. In contrast, at the other end, there are those who consider experts as fully rational, in the sense that experts are always able to justify their actions (Montero & Evans, 2011). With such view, intuition is a trait that is rather associated with non-experts. Between those two extremes, there are researchers who view intuition as an integral component of expertise (Gobet & Chassy, 2009; Gobet & Simon, 1996; Newell & Simon, 1972). While these scholars do not equate intuition with expertise, they acknowledge it as a significant building block in the development of expertise.

To better understand the differences between these theories, it is helpful to consider their origins, i.e. the research traditions from which they emerged.

Within cognitive psychology, Newell and Simon (1972) were the first ones to propose a model of intuition within their broader theory of human problem solving. At the core of their theory lies the concept of *bounded rationality*, suggesting that experts and novices grapple with the same cognitive constraints: we can only focus our attention to one thing at the time and we can only hold up to four items in our visual short-term memory (Simon, 1982). If human cognition, and our ability to be rational, is inherently bounded, how do we explain situations where individuals arrive at the correct solution in a shorter time than would be required through complete analytical thinking? Newell and Simon (1972) suggested that this is because small pieces of knowledge can be ‘chunked’ into larger entities. According to this *chunking theory*, intuition is the same as pattern recognition, while expertise is a combination of pattern recognition (intuition) and selective search through the states of a problem space.

While Newell and Simon were cognitive psychologists who wanted to describe intuition in terms of its underlying cognitive processes (i.e. focusing on the components of intuition), Herbert Dreyfus was a philosopher who wanted to provide a phenomenological description of intuition (emphasising the holistic nature of intuition).

Dreyfus and Dreyfus (1986) criticised chunking theory for defining the types of chunks in isolation from any contextual considerations, thus contradicting their holistic view of intuition and expertise. In response to this criticism, Gobet and colleagues proposed *template theory* (Gobet & Chassy, 2009; Gobet & Simon, 1996), according to which chunks that frequently recur in a specific environment can turn into larger cognitive structures known as *templates*. Each template consists of a *core* of stable information corresponding to the original chunk, and a *slot* for encoding variable information. Overall, information processing within a template is fast as it consists of chunks and associations that have occurred many times before. By extending chunks to templates, Gobet and colleagues (Gobet & Chassy, 2009; Gobet & Simon, 1996) were able to reconcile the holistic nature of intuition, while maintaining the option to dissect intuition into smaller components.

Although the above-mentioned scholars held contrasting views on many aspects of intuition and the development of it, their theories had one thing in common – they primarily built on studies of *expert* intuition. This differs from my work, in which I am more interested in what I refer to as *novice intuition.*

3.4.1 Intuition in education

Before proceeding to how intuition has been studied in the context of problem solving within CER, it is important to note that while Dreyfus and Dreyfus, Montero and Evans and Simon and colleagues, did not primarily focus on novice intuition, they have all offered insights into the implications of their theories for education.

Dreyfus and Dreyfus (1986) posited that since intuition is a holistic quality, it has to be acquired in a holistic manner. From this perspective, the development of intuition in novices requires exposure to real-world scenarios, where they can accumulate procedural knowledge (know-how) and gradually transition into experts. Such an approach places a strong emphasis on learning through hands-on experience and solving problems in authentic contexts.

By contrast, Montero and Evans (2011) conclude that it should be possible to extract heuristics from experts and then teach them to students through explicit instruction and feedback. Since they believe that expert intuition is rational and can always be justified, it should also be possible to extract heuristics from experts and then teach them to students through explicit instruction and feedback.

Finally, proponents of template theory (Gobet & Chassy, 2009; Gobet & Simon, 1996), suggest a combination of these approaches. Experts leverage both their know-how and know-that to navigate during problem solving. While know-that may be transmitted through explicit instruction, know-how often requires hands-on experience in specific contexts. Facilitating the latter might involve scaffolding and adjusting the degree of openness in tasks.

In summary, the educational implications of these theories reflect distinct approaches, with Dreyfus and Dreyfus emphasising experiential learning, Montero and Evans advocating for explicit and rule-based instruction, and template theory offering a middle-ground perspective.

Before concluding this section, I would like to underscore that there exists a wealth of additional interpretations of *intuition*; vague concepts often resist precise definition and many have attempted to pin down its 'true' nature. Given the constraints of this thesis, I will now present a final perspective.

Within mathematics education research, Brady et al. (2022, p. 217) have proposed that 'at any expertise level, a person's tacit knowledge system can give rise to rapid interpretations of their surroundings, enabling them to act fluently and with confidence (even if the interpretations or actions are flawed)'. This definition does not exclude novices from having intuition, rather it emphasises that all individuals exist at their own *current* level of expertise and can act intuitively based on that level of expertise.

3.4.2 Intuition in CER: the role of heuristics

Within chemistry education research (CER), the development of intuition has primarily been approached through the investigation of heuristics. Heuristics can be thought of as simple rules, allowing problem solvers to move forward without having to engage in full analytical problem-solving strategies (Kahneman, 2011). The role of heuristics in human reasoning has long been debated by researchers in the field of psychology, with the discussion being dominated by two views: *dual-processing theory* (DPT) as proposed by Tversky and Kahneman (1972, 1982) and the *adaptive toolbox* (AT) as proposed by Gigerenzer and Todd (1999).

According to DPT, the human mind operates through two systems, or types of processes: system 1 (type 1 processing) is fast and intuitive, while system 2 (type 2 processing) is slow and analytical. Although we rely on both systems when making sense of the world, our first impression of a situation is typically governed by fast, type 1 processing.

Early research efforts on the differences between system 1 and system 2, yielded ample evidence suggesting that type 1 processing was prone to errors and biases, emphasising the importance of system 2 as a means to correct the mistakes made by system 1. This eventually earned system 1 a somewhat negative reputation, sparking debates on whether educators should steer students towards minimising their reliance on type 1 processing in favour of type 2 processing. Today, most researchers agree that there is not such a dichotomy and that labelling system 1 as 'the bad guy' was never Kahneman's intention. The question is not whether we should exclusively rely on type 1 or type 2 reasoning; both types will always be present in our minds. The question is rather *when* to depend on one over the other.

Advocates of the AT (Gigerenzer & Gaissmaier, 2011; Gigerenzer & Todd, 1999) have criticized DPT precisely because of the negative connotation that was given to heuristics, proposing instead that we think of the human mind as a collection of heuristics that can be combined in different ways to solve specific tasks in specific environments. They refer to this collection of heuristics as *the adaptive toolbox*.

Numerous heuristics have been proposed in the literature. Typically, a full characterization of a heuristics consists of empirical evidence, a qualitative description and a statistical model. The most common heuristics to discuss in relation to students' decision-making approaches during problem solving are: *the recognition heuristics*, i.e. a decision is based on the recognition of an object; *the representativeness heuristic*, i.e. a decision is made assuming commonalities between objects of similar appearance; and *the one-reason heuristic*, i.e. a decision is based on the first cue that favours one alternative over the others (Gigerenzer & Gaissmaier, 2011).

Within CER, Talanquer and colleagues have conducted extensive work on what heuristics that are employed by chemistry students while making decisions about acid strength (McClary & Talanquer, 2010), and what implicit assumptions that constrain students' cognition (Maeyer, 2013; Maeyer & Talanquer, 2010, 2013). In their work, they rely on concepts from both DPT and AT, adopting DPT to discuss intuitive and analytical reasoning (type 1 and type 2 processing) in combination with some of the heuristics proposed by AT for inductive data analysis.

Employing the same theoretical underpinnings, Graulich and colleagues have investigated students' intuitive judgments and use of heuristics in the context of organic chemistry (Graulich, 2014; Graulich et al., 2010).

Researchers in CER and PER seem to agree that the relationship between intuitive and analytical reasoning is mutual; to be able to navigate uncertain situations, a problem solver should engage in intuitive *and* analytical thinking. The challenge lies in finding a good balance. This is easier said than done, and experts have been shown to be better than novices at optimising which process to rely on when. Scholars now suggest that the development of metacognitive competence should be a fruitful way to help students balance between intuitive and analytical strategies (Graulich, 2014; Kryjevskaia et al., 2021; McClary & Talanquer, 2010).

3.5 Laying the theoretical basis for my thesis

The preceding sections briefly outlined the potential contributions of the mentioned theories and frameworks to the theoretical underpinnings of my research project. Herein, I articulate the specific assumptions from each theory and analytical framework that form the theoretical framework of my thesis

Cognitive science asserts that it is possible to gain insights into an individual's mind by examining their actions and the manner in which they execute them. This assumption, along with various concepts of *speech* within **sociocultural theory** (i.e. social and private speech), has informed my choice of method for the data collection, i.e. think-aloud problem solving and follow-up interviews.

Constructivism posits that learners build on their previous experiences when acquiring new knowledge. This viewpoint is reflected in my choice to adopt a *resources perspective*.

The resources framework further contributes with a definition of knowledge as comprised of small cognitive units or *resources*. This perspective should facilitate the characterisation of extra-mathematical knowledge by allowing a deeper exploration into the nuances of the extra-mathematical realm. Moreover, it enables the examination of students' problem-solving approaches in terms of framing and resource activation. Such analysis could potentially be helpful in uncovering what factors that contribute to productive or unproductive activation of resources, shedding light on the conditions for successful problem solving at the interface of chemistry and mathematics.

Problem-solving concepts relevant to this thesis are *deep and superficial procedural knowledge* as defined by Star (2005, 2007) and *Goos's metacognitive pathways* (1998, 2002). These concepts are important for the discussion of Paper II, where I delve deeper into the extra-mathematical factors that influence students' decision-making during problem solving.

The mathematical modelling cycle (MMC) comes with two potential contributions to my work.

Firstly, it offers a comprehensive description of the processes involved in mathematical modelling of real-world situations, including a structure for how these processes are interrelated. Since I am interested in studying how students approach chemistry problems that require some degree of mathematical modelling, the MMC's processes and structure should serve as helpful starting points for analysing and organising our research data.

Secondly, the MMC explicitly recognises the importance of extra-mathematical knowledge (EMK) for certain processes. Given that knowledge in chemistry falls within the realm of EMK, focusing the analysis on processes that require EMK will provide valuable insights into how chemical and mathematical knowledge interact during modelling activities. Furthermore, while

EMK has been differentiated from mathematical knowledge, its own attributes and elements have received limited attention, leaving the extra-mathematical realm largely unexplored. Thus, by delving into the details of the extra-mathematical realm, my research has the potential to make significant contributions also to the broader field of mathematical modelling.

Finally, I adopt a definition of **intuition** in accordance with Brady et al. (2022), thus asserting that any individual can act intuitively based on their tacit knowledge which corresponds to *their current level of expertise*. I find this definition promising for the discussion of how students develop intuition.

4 Research questions

The overarching goal of this licentiate thesis is to explore how students engage in problem solving at the crossroads between chemistry and mathematics, with a special focus on the context of chemical kinetics where problem solving is known to involve challenging translations and transitions between chemical phenomena and mathematical representations.

Against the background provided by the literature review (Chapter 2) and my theoretical framework (Chapter 3), Paper I set out to answer the following research questions:

- **RQ1:** How can the MMC be refined to provide a framework that allows us to capture and analyse, at a higher level of resolution, the specific processes that students engage in while solving a problem in chemical kinetics?
- **RQ2:** When and how do students use extra-mathematical input during the problem-solving process and what roles do such input play?

Building on the results from Paper I, Paper II was guided by the following research questions:

- **RQ1:** How can the nature of *other resources* be characterised in more detail?
- **RQ2:** What roles do *other resources* play during problem solving at the crossroads between chemistry and mathematics?

5 Methodology

In this chapter, I outline the methodology employed to explore the research questions of my thesis. First, I present the overall methodological approach – *a theory-informing subjectivist inductive approach* (Section 5.1). Subsequently, I introduce the specific research methods employed in collecting and analysing the data – *think-aloud techniques and semi-structured interviews* and *thematic analysis* (Section 5.2). The next section includes a brief account of how trustworthiness is generally established in quantitative and qualitative research, how it is commonly established within CER, and finally, how it has been established in this thesis (Section 5.3). In the concluding section, I discuss the ethical considerations of my two research studies (Section 5.4).

5.1 Subjectivist inductive approach

To explore the research questions of this thesis, I have adopted a qualitative research methodology (see also Section 2.1.2.2) that combines a *subjectivist inductive approach* with *theory-informing data analysis,* resulting in a *theory-informing data analysis subjectivist inductive approach* (phew!). In the following sections, I break down this rather lengthy label, starting at the end.

Inductive and deductive approaches. The approach to a research study can be described as either *inductive* or *deductive*, depending on how the researcher moves between data and theory. An *inductive*, or 'bottom-up,' approach describes a process of going from something specific to something more general, i.e. *from data* to theory. Thus, a researcher adopting an inductive approach starts by collecting data, looks for patterns within the data, and then formulates a theory capable of explaining the observed patterns. A *deductive* ('top-down') approach describes a process moving in the opposite direction, i.e. *from theory* to data. This means that a researcher embracing a deductive approach begins with a well-established theory and applies that theory to interpret and analyse data (Cohen et al., 2018).

To further illustrate this dichotomy, I find the famous line sung by the Irish rock band U2, 'I still haven't found what I'm looking for', to effectively convey the essence of a deductive approach, implying a quest for something predefined (e.g. the principles of some theory). Most scientific investigations are deductive in the sense that they rely on some existing theory to generate and test hypotheses. In contrast, an inductive approach is better captured by the phrase: ‘I’m not really sure what I’m looking for’, suggesting an exploratory journey with a less clearly defined direction.

Given that, at the outset of my first research study, I was not entirely sure about what I was looking for, it seemed appropriate to approach my research questions inductively.

Subjectivism and objectivism are two distinct philosophical perspectives that differ in their views on the nature of reality, truth, and knowledge. Within educational research, our primary concern revolves around the nature, scope and limits of knowledge: a field known as *epistemology*. As such, the remainder of this section will focus on outlining the epistemological standpoints of the two perspectives (Varpio et al., 2020).

Subjectivism holds that knowledge is rooted in personal experiences, feelings, and interpretations. Consequently, subjectivists argue that multiple truths exist (i.e. that truth is subjective) and that individuals construct their own understanding of reality. In contrast, *objectivism* asserts that there is a reality that exists independently of individual perceptions, and that objective truths can be discovered through systematic inquiry and reasoning. While subjectivism is often associated with an inductive research approach, objectivism is more commonly associated with a deductive approach.

In my exploration of students’ problem-solving behaviours, I have adopted a subjectivist inductive approach. This choice was motivated by evidence of problem-solving behaviours being highly individual (students ‘bounce around’ in the mathematical modelling cycle) and dependent on students’ prior experiences as well as their expectations of the problem-solving situation.

The role of theory in subjectivist inductive research. As mentioned above, adopting an inductive approach means going from data to theory, with theory emerging as a product of the research. Adding to this the subjectivist view of theory as constantly evolving, allows the *subjectivist inductive* researcher to draw upon existing theories in their pursuit of theory development. According to Varpio et al. (2020), subjectivist inductive approaches can be divided into three categories based on whether, and how, existing theories are leveraged.

The first category, labelled *fully inductive theory development*, corresponds to an approach where the researcher explores the research topic with a ‘blank slate’, devoid of any pre-conceptions. Theory is generated solely from patterns and themes emerging from the data, and remains uninfluenced by the researcher’s prior experiences and/or values; theory is the *product* and no pre-existing theory is used to inform the study design. This approach is frequently adopted by scholars within the grounded theory tradition (Varpio et al., 2020).

Conversely, in a study adopting a *fully theory-informed* inductive approach, theory plays a central role in shaping the entire research process. A theoretical framework is articulated at the outset of the inquiry, guiding every aspect of the research process, from study design to data collection and analysis.

Similarly, a *theory-informing data analysis* inductive approach involves the researcher holding multiple theories in mind at the beginning of the study. However, this approach also allows for insights emerging from the data to influence and shape the final theory, meaning that the development of the theoretical framework takes place alongside the data analysis. The approach is iterative and essentially alternates between a deductive approach, relying on the preliminary framework to analyse the data, and an inductive approach, modifying the theoretical framework as new insights emerge during iterations of analysis (Varpio et al., 2020).

Researchers adopting this kind of approach often refrain from determining which theories will be applied in the final round of data analysis until preliminary analyses are underway. Along the way, the preliminary theoretical framework guides the research design. Notably, the theoretical framework guides *only certain aspects* of the research design. Therefore, it is crucial for the researcher to clearly outline which aspects of the design that are informed by theoretical assumptions and in what way.

At the beginning of my research journey, I thought that I was going to use a *fully theory-informed* inductive approach, i.e. that I would select a theory, or perhaps multiple theories, at the outset of my work that I would later employ to analyse my research data. Eventually, I realised that my research topic was far too open and ill-defined to be subjected to such methodology. After all, there was no well-established model for analysing problem solving at the interface of chemistry and mathematics, and (close to) all I knew was that we (i.e. my supervisors and I) were keen to explore the interaction between students' knowledge of chemistry and mathematics. Thus, it turned out that adopting an inductive approach employing *theory-informing data analysis* was a much better option for the purpose of exploring my research topic, allowing my theoretical framework to evolve as new insights emerged from my data analyses.

5.2 Research methods

In this section, I present the research methods that were employed in collecting and analysing the data discussed in this thesis. I begin, however, with an overview of the research participants and the research setting.

5.2.1 Research participants and setting

The participants taking part my research studies were all second-year students majoring in chemistry or chemical engineering. At the time of data collection, these students were enrolled in introductory course in physical chemistry, which featured a dedicated module on chemical kinetics. Prior to this course, the students had completed a mix of introductory courses in chemistry (general, organic and inorganic chemistry) and mathematics (linear algebra and geometry and single variable calculus).

This particular group of students was deliberately selected to ensure that participants had some prior knowledge of the concepts central to the tasks employed in the data collection. Moreover, the introductory physical chemistry course is considered an upper-level course as it is given during the students' second year at university. As highlighted in Section 2.3, upper-level courses are relatively underexplored within CER, thus making this research cohort particularly interesting.

The recruitment process is outlined in Section 5.4.3.

5.2.2 Data collection

Research data were collected during problem-solving sessions where students worked together in pairs to solve a set of tasks centred around a key concept in chemical kinetics. The problem-solving sessions were video recorded and a *think-aloud protocol* was employed to follow the students' reasoning.

While I prefer to call this method *think-aloud problem solving*, I have found that within the CER literature, this method is commonly referred to as a *semi-structured interview,* using a *task* as the structuring component and a *think-aloud protocol* to capture students' thinking (Bretz, 2008; Cowan, 2019; Watts & Finkenstaedt-Quinn, 2021). Thus, in this section, I explain what is meant by *think aloud* and acquaint the reader with the *interview* as a qualitative method for data collection.

5.2.2.1 Think aloud

Using a think-aloud protocol for gathering research data involves asking the participants to verbalise their thoughts while engaging in a specific task or activity and observing their behaviours (Cowan, 2019).

The researcher may opt for direct observation of the participants, or record their actions (typically through video and/or audio recordings) for subsequent analysis. Often, a combination of direct observation and recordings is used to capture as many nuances of the situation as possible. Moreover, by providing real-time insight into participants' behaviours during the task, direct observation enables the researcher to inquire about particularly noteworthy occurrences in follow-up interviews. In such way, direct observation allows for a more in-depth exploration of students' thoughts, reactions, and motivations, thereby enhancing the overall richness of the collected data.

Since the chosen task or activity will guide the direction of the session, think-aloud methods are considered interventionist as opposed to naturalistic. Simply put, this means that the situation is constructed rather than natural; the observations are influenced by the researcher's choice of task and are likely to deviate from the normal (or natural) behaviour of the participants (Taber, 2013).

Nevertheless, think-aloud techniques serve as valuable tools for gaining insights into participants' cognitive processes. It is, however, important to understand that think-aloud methods can only capture cognitive processes that participants are consciously aware of. Another limitation is that the method is compatible only with tasks that allow for participants to articulate their thoughts during performance. It might therefore be difficult to collect think-aloud data with tasks that impose a high cognitive load on participants. In such cases, *stimulated recall* might be a more suitable option (Taber, 2013).

Stimulated recall is a method that consists of two phases. In the first phase, the participants are video recorded while engaging in a task. However, they are not required to verbalise their thoughts. In the second phase, the participants get to watch the recording of themselves performing the task and are subsequently interviewed by the researcher about their thoughts and feelings at various specific moments in the recording. In that way, stimulated recall allows participants to share their reflections after completing a task.

5.2.2.2 Interviews

The interview is a frequently used method in qualitative research. Providing a platform for direct interaction, it enables researchers to delve into the diverse perspectives, experiences and interpretations of the participants involved. The quality of data generated through interviews depends on several factors such as the experience and positioning of the interviewer, the structure of the interview and the participant/interviewee composition. In the subsequent sections, I delve into how various aspects of these factors pertain to data quality.

The interviewer. There are different ways in which the interviewer may affect the quality of the data. For instance, the interviewer's experience level is likely to affect their ability to 'ask the right questions' and facilitate a smooth and natural conversation. Another important aspect of the interviewer is their positioning as either an insider or outsider in relation to the investigated context.

An *insider* refers to someone with direct experience of, or belonging to, the same community or group as the interviewee. Sharing a common language and cultural understanding with the interviewee may facilitate trust-building and the exploration of sensitive topics. Furthermore, an insider might pick up on nuances that may be overlooked by an outsider. There are, however, certain drawbacks of having an insider position such as assuming shared knowledge and thus, miss out on important details that an outsider might react to and inquire about. Thus, bringing ‘fresh eyes’ to the situation, an *outsider* may ask more objective questions, challenging preconceived notions and norms that are taken for granted by the insider. On the other hand, an outsider might find it challenging to establish trust. Additionally, an unfamiliarity with the context might give rise to more misunderstandings (Kvale & Brinkmann, 2014).

The structure of the interview. An interview can be open, semi-structured or structured. *Open interviews* are flexible and exploratory in nature. No questions are planned beforehand and the interview is more or less guided by the interviewee with the researcher acting mainly as a facilitator. Open interviews are generally time consuming, making them suitable for studies aiming to gain rich and deep insights into a few numbers of individuals.

In contrast, *structured interviews* are highly organised, with the researcher employing a pre-determined interview protocol to make sure that each research participant is asked the same set of questions. This kind of interview is similar to a questionnaire and frequently employed to gather comparable data for quantitative analysis.

Finally, there are *semi-structured* interviews. They resemble open interviews in that they are flexible and exploratory. However, the researcher typically relies on interview guide containing a set of core questions to provide the conversation some structure and direction. This kind of interview is often used when the researcher is keen to explore certain key topics but also wants the interviewee to be free to take the conversation in unexpected directions. In order for semi-structured interviews to function well, it is crucial for the researcher to be alert and adapt to participant responses (Kvale & Brinkmann, 2014; Robson & McCartan, 2016).

The participant composition. The three most commonly used participant compositions are individual interviews, interviews in pairs, and group interviews. While the *individual interview* is excellent for gaining in-depth insights into an individual’s experiences and thoughts, it is a highly constructed situation, making it less suitable for interviews where there is a pronounced power imbalance. For instance, a child being interviewed by an adult might feel uncomfortable sharing their inner thoughts in an individual interview. The same goes for a student being interviewed by a teacher or some other authoritative figure. It is worth noting that the power dynamics can also tip in the opposite direction; the interviewee might hold a higher position than the interviewer.

In the presence of a power imbalance, opting for *interviews in pairs* or *group interviews* may be preferable. The advantages of such interviews include allowing for more natural conversations and being more efficient in quickly gathering a larger amount of data. However, they do come with certain disadvantages. For example, interviewees may adapt their responses to each other, potentially resulting in more superficial data. This tendency is likely more prevalent when interviewees do not know each other well. If they know each other well, other challenges may arise, such as assuming shared knowledge and thus omitting details that remain unknown to the interviewer. Furthermore, data analysis can be challenging, especially when interviewees talk simultaneously (Kvale & Brinkmann, 2014; Robson & McCartan, 2016).

Summary. Importantly, the impact of these factors on the overall quality of the data depends less on their intrinsic characteristics and more on how well they align with the rest of the research design: whether the goal is to explore in-depth perspectives or capturing a broader range of experiences, the nature of the relationship between the interviewer and the investigated context, and the nature of the relationship between the interviewer and the interviewee, and so on.

5.2.2.3 General method for data collection in my research studies

I refer to the general data collection method used in the research studies presented in this thesis as *think-aloud problem solving* (also referred to as *semi-structured interviews* centred around a *task* and combined with a *think-aloud protocol*). Herein, I provide the rationale for selecting this particular approach.

The structure of the problem-solving sessions. Data collection began about a week after the students had completed the lecture series on chemical kinetics in their physical chemistry course. Each student pair took part in a problem-solving session with two distinct phases: in Phase I (~ 45 minutes) students worked on the tasks without any guidance from the researcher; in Phase II (~ 25 minutes) the researcher took a more active role, discussing the tasks together with the students, thus making room for clarifications concerning the tasks and the study as a whole.

The tasks were printed out on individual sheets of paper and presented one at a time. In addition, a printed-out reaction mechanism was made available to the students throughout the session. The students worked consecutively with the tasks and were free to choose when they were satisfied with their work on a task. They could then reveal and start working on the next task.

The tasks used in each problem-solving session. Research participants were asked to solve a set of six tasks centred around a central concept in chemical kinetics (i.e. *the steady-state approximation, SSA*). The tasks were designed to require varying degrees of integration of chemistry and mathematics in order to be solved. One of these tasks, Task 4 (Appendix I), was expected to require a much higher degree of interaction between chemistry and mathematics as compared to the other tasks. Consequently, Task 4 became the focus of the data analyses in both papers.

Think-aloud problem solving. A think-aloud protocol was employed to capture the students' reasoning during problem-solving sessions where they engaged with tasks in chemical kinetics. The students' writing and hand gestures were video-recorded as they were expected to point to various parts of the printed-out reaction mechanism. In addition to video recordings of the discussions, a Livescribe™ smart pen was utilised to document the students' note-taking while simultaneously recording the audio of their dialogues (Linenberger & Bretz, 2012).

The decision to adopt this method aligns with the theoretical underpinnings of this thesis, with cognitivism positing that *it is possible to gain insights into an individual's mind by examining their actions and the manner in which they execute them* and sociocultural theory asserting that *language enables learners to articulate their thoughts both to others and themselves*.

Observation of *pairs*. During the recruitment process, participants were asked to sign up for the study in pairs. Each pair was then observed while collaborating on a problem-solving activity. The decision to have the participants sign up with someone of their own choosing, and subsequently observe them working together, was made with the intention to create a more natural and relaxed environment. The idea was that such a setting would encourage students to articulate their thoughts and express themselves more freely compared to thinking aloud individually. Moreover, providing students with the opportunity to share and test various ideas and problem-solving ideas with each other was anticipated to yield a more diverse and richer set of data.

The background and positioning of the interviewer. In all problem-solving sessions conducted for my studies, I assumed the role of the interviewer.

Having previously completed the same introductory course in physical chemistry (as the one attended by the students), I was already acquainted with most parts of its structure and content. However, considering that a decade had passed since I attended the course, I took the initiative to sit in on relevant lectures before the first data collection period. This allowed me to familiarise myself with the educational material that students would have encountered prior to the problem-solving sessions, increasing my chances of adopting an insider perspective.

I initiated each problem-solving with some casual conversation, asking the students about their day, their current courses, and how they were feeling about life and university in general. This initial phase took the form of 'small talk' rather than a formal interview, and there was no pressure on the students to respond to my questions. To create a fair exchange, and potentially bridging the gap between insider and outsider perspectives, I also shared information about my background, highlighting that I had been a chemistry student at Uppsala University as well and that this had eventually led me to pursuing a PhD in chemistry education research. The intention behind the small talk was to foster a relaxed atmosphere, making sure that the students understood I was not there to judge their performances but merely to observe and gain insight into my research topic.

During Phase I, when the students worked without any guidance from me, I positioned myself in a way that kept me out of their immediate line of sight as a means to minimise any influence on their behaviour. My intention of being present in the room was to take field notes, capturing key events that would serve as the foundation for an interview guide to be utilised in Phase II.

Adding to this, it should be acknowledged that the language used during data collection was *Swedish*, and that consequently, the transcriptions were in Swedish as well. However, considering that the theories I relied on were typically conceptualised in English and since I consistently employed deductive coding as a first step of the thematic analysis, I recently realised that despite my data being in Swedish, my codes were all in English. Although having to translate between languages could potentially increase the risk of misunderstandings, especially across authors, I do not believe this to be a problem in this particular case, as all authors in both papers can be considered fluent in both Swedish and English.

Some excerpts of students' dialogues were selected for translation and publication.

5.2.3 Data analysis

Data analysis is the process of turning raw data into findings. Whether to subject the data to quantitative or qualitative data analysis depends on various factors such as the nature of the data, the size of the dataset, and the purpose of the research (see Section 2.1.3).

Since the aim of my research is to gain a deeper understanding of a rather unexplored phenomenon, I have opted for a *qualitative* data analysis method.

In the upcoming section, I acquaint the reader with the general process of qualitative data analysis and outline the specific methods employed in the analyses conducted in my research studies.

5.2.3.1 Qualitative data analysis

> There is no single or correct way to analyse and present qualitative data; how one does it should abide by *fitness for purpose* [emphasis added].
>
> (Cohen, 2008, p. 643)

Qualitative data analysis (QDA) is the process of transforming the data of a studied phenomenon into rich descriptions, explanations and interpretations (Cohen 2008). The ultimate goal of QDA is to gain a deep understanding of the event under investigation. Typically, this involves: (1) preparing the data for analysis; (2) formulating a coding scheme; (3) analysing the data using the coding scheme; and (4) evaluating the findings in relation to the research questions. However, various QDA methods exists, and depending on their focus, goals, and level of interpretation, the details and specific order of the aforementioned steps may vary (e.g. Bingham, 2023; Vanover et al., 2021).

For instance, *content analysis* primarily aims to reveal trends, patterns and correlations through quantifying the content of the data. While this method can be applied to both quantitative and qualitative data, its application to the latter essentially involves turning qualitative data into numbers corresponding to the frequency of certain predefined categories or concepts. The predefinition of categories implies that the development of the coding scheme (step 2 above) typically starts with a deductive approach. In contrast, *thematic analysis* seeks to uncover and make sense of the meanings embedded in qualitative data. The explorative nature of such endeavour makes it more suitable to begin the construction of the coding scheme (step 2 above) in an inductive manner. Other common QDA methods include grounded theory analysis, narrative analysis and discourse analysis. As eloquently put by Cohen (2008, p. 643), the choice of method should be assessed with respect to the research objective.

In the following sections, I provide more details on each of the key steps mentioned above. In my research studies, I have employed *thematic analysis*.

Step 1: Preparing the data for analysis. In the first stage, the researcher prepares the data to facilitate the subsequent analysis. This typically involves transcribing recorded visual and/or auditory data into textual such, formatting the text for improved readability, adding time stamps, and other relevant tasks. Additionally, the researcher may write a summary based on a preliminary analysis and field notes gathered during the data collection. While the primary aim of this stage is to generate organised, manageable, and searchable data, i.e. to create a document that lends itself to analysis, it also serves as an opportunity for the researcher to become familiar with the data (Cohen, 2008).

Step 2. Formulating a coding scheme. Once the data has been organised into a manageable and well-structured text document, the researcher can begin the process of *data reduction*. That is, reducing the complexity of the data, often through several iterations of *coding*. In qualitative research, coding entails labelling, categorising and grouping data as a means to reveal patterns and trends. The purpose of data reduction is quite well captured by the expression 'can't see the forest for the trees', which signifies that focusing too much on details or individual components can make it difficult to grasp the 'bigger picture'. Importantly, data reduction should be performed such that the quality of the qualitative data is maintained (Cohen, 2008). In other words, the final coding scheme should comprise just enough codes to capture the essence of the phenomenon being studied, neither more nor less. Two strategies can help achieve this balance.

The first strategy involves adopting an iterative approach, alternating between two distinct modes of analysis: deductive and inductive. As mentioned above, which mode is best suited for the first phase of the data reduction varies between methods. However, whenever using a method with an initial theoretical framework, it is often beneficial to start with a deductive approach. That is, to rely on predefined categories and concepts outlined in the theoretical framework in analysing the data. In such a way, the data will be reduced into a subset of codes (i.e. an initial coding scheme) reflecting the research questions and the purpose of the research (Cohen, 2008). Inductive analysis can then be applied to extend and modify the initial coding scheme based on insights and themes emerging from the data.

The second strategy is to engage in the process of *constant comparison*. This involves, on the one hand, systematically comparing existing codes with each other to identify similarities and differences, potentially leading to the combination or disregard of unreliable codes. On the other hand, it also entails continuous comparison of the coding scheme with new codes emerging from the data, possibly resulting existing codes being refined or revised to increase the consistency with which they are applied (Strauss & Corbin, 1990).

Notably, these two data reduction strategies take place concurrently rather than sequentially, continuing until no new codes, categories, or themes emerge from the data. At that point, the coding is said to have reached *saturation* (Saunders et al., 2018).

Step 3. Analysing the data using the coding scheme. Once the final coding scheme has been established, the data can be coded and analysed according to the research questions. At this stage, the focus is not on searching for patterns in order to create new codes; instead, researchers examine patterns within the *coded data* as a means to make sense of it from a broader perspective. The aim is to answer the research questions and provide valuable insights that may fulfil the research objective. The outcome of this stage is the findings of the analysis (Cohen, 2008).

Step 4. Evaluating the findings with respect to the research questions. In the final step, the findings are evaluated in relation to the entire conceptual framework. This includes the research questions and objectives, the literature review and the theoretical framework (Cohen, 2008).

5.2.3.2 Developing coding schemes for my research studies

As previously outlined, my research is partly grounded in the principles of cognitive science and sociocultural theory, thus assuming that insights into learners' cognitive processes may be inferred from their verbal expressions. Consequently, while video data offers both visual and auditory information, enabling analysis of participants *actions* as well as their *talk*, I have primarily focused my analyses on the latter. In the following sections, I provide an overview of how these analyses were carried out.

Firstly, I transcribed and organised the recorded video data, preparing it for subsequent *thematic analysis*. Accordingly, each analysis involved iterative cycles of *deductive coding*, using concepts and ideas from the theoretical framework to organise the data, and *inductive coding*, allowing themes and insights emerging from the data to also inform the development of the final coding scheme. All stages of the data analyses, including transcription and coding, were carried out manually in NVivo® (NVivo Qualitative Data Analysis Software). Although time-consuming, this process provided me with an excellent opportunity to familiarise myself with the data. While I conducted the transcriptions entirely on my own, the whole research team participated in the construction of the final coding scheme.

The development of the coding scheme consisted of three distinct ‘rounds’ of analysis. In the first round, one of my co-authors and I independently coded a given portion of the data. During the second round, we met to compare our coding attempts and discussed discrepancies until we had agreed on an initial coding scheme. In the third round, the entire research team scrutinised the coding scheme. This third round was repeated and became the *final* round of analysis only when the whole team had reached a consensus on a final coding scheme and saturation had been achieved (Saunders et al., 2018). These three rounds could also be described as two waves of *negotiated agreement*.

Importantly, the co-author who took part in the first round of the analysis also served as the teacher for the module on chemical kinetics attended by the research participants. While this circumstance could have potentially influenced the interpretation, leading for example to assumptions that the students possessed more knowledge than explicitly demonstrated (i.e. the teacher assuming shared knowledge because of their insider position in this particular situation), it also facilitated the coding of certain parts of the transcripts where students referred to highly specific events that occurred during class. I believe that our implementation of negotiated agreement during the first round of analysis helped mitigate the aforementioned concern.

5.3 Trustworthiness and reliability

> … incorporating clear demonstrations of the steps taken to establish the reliability of qualitative analyses in CER will ultimately serve to *strengthen the rigor of the field* [emphasis added] so both researchers and practitioners can make better sense of the ways they can incorporate key findings and results into their own future research or instructional practice.
>
> (Watts & Finkenstaedt-Quinn, 2021, p. 574)

Trustworthiness refers to *the quality of being trustworthy*. In everyday life, a trustworthy individual is someone who is honest and truthful: simply put, a person you can trust. Essentially, these terms bear the same meanings when applied in the realm of research; trustworthy work can be trusted, and achieving a high level of trustworthiness involves an honest and truthful presentation of the research findings as well as the research design, thus emphasising the importance of transparency.

The insightful words by Watts and Finkenstaedt-Quinn (2021, p. 574) articulate the importance of transparency in establishing trustworthiness in CER, highlighting its dual role to: ‘strengthen the rigor of the field’ by ensuring that research findings are meaningful, reliable, and credible; and promote the realisation of findings in research as well as practice.

In the subsequent sections, I explore how trustworthiness is established in quantitative and qualitative analysis, how it is typically established within the context of CER, and how my co-authors and I have established trustworthiness (or reliability) in the work presented in this thesis.

5.3.1 Trustworthiness in quantitative and qualitative research

While trustworthiness is crucial to both quantitative and qualitative research, the manner in which it is established differs between the two paradigms.

In quantitative research**,** trustworthiness is typically assessed through *internal validity, external validity, reliability,* and *objectivity*. These metrics are widely used to evaluate trustworthiness in ‘pure science’ and other fields that lend themselves to a positivist and rationalistic research paradigm.

Table 1. Overview of naturalistic criteria and rationalistic metrics, and how they relate to each other.

RATIONALISTIC	NATURALISTIC
Internal validity reflects the *accuracy* of the research design and the selected methodology. It measures the accuracy of the whole research apparatus in itself, answering the question: does it really measure what it is intended to do?	**Credibility** concerns the *accuracy* of the data and whether it has been collected and analysed in a way such that it really corresponds to ‘reality’. Two examples of how to increase credibility are member-checking and triangulation.
External validity relates instead to the accuracy in relation to other contexts. Often discussed in terms of *generalisability*, it answers the question of whether the research findings can be generalised to other, external, contexts.	**Transferability** is the naturalist’s version of generalisability. Since naturalists do not aim to discover context-free truths, generalisability is rarely in their interest. Nevertheless, they believe that rich descriptions may facilitate the *transfer* of research findings from one context to another.
Reliability concerns the consistency and stability of the methods used in a study. A crucial aspect of reliability is that of *reproducibility,* i.e. whether the research methods are capable of generating consistent results over time.	**Dependability** is related to reliability in that it captures the consistency and stability of the research process, ensuring that the findings are replicable and reliable. It is often demonstrated by engaging a qualified person in an inquiry audit and through clear documentation (transparency).
Objectivity underscores the need for research to be *unbiased*, emphasising the importance to minimise the impact of the researcher’s personal bias in data collection and analysis.	**Confirmability** refers to the degree to which the findings of a study are shaped by the participants and their contexts (i.e. the data) rather than the researcher’s personal biases. This can be achieved through practicing reflexivity, i.e. reflecting on one’s own biases and how they may influence the research process.

Although some scholars insist that the same quantitative measures should be used to assess trustworthiness in qualitative research, others suggest a more naturalistic approach focusing on *credibility, transferability, dependability,* and *confirmability,* as laid forward by Lincoln and Guba (1985). These naturalistic criteria relate to the rationalistic metrics as outlined in Table 1.

5.3.2 Establishing trustworthiness in CER

A persistent challenge in CER is the fact that the literature and its intended audience are often rooted in different research traditions. While the majority of qualitative CER studies align with a subjectivist tradition, many practitioners, especially at the university level, are more familiar with the objectivist approach to research and its associated criteria for trustworthiness. To bridge this gap, Watts and Finkenstaedt-Quinn (2021) encourage scholars in CER to frame discussions of trustworthiness in terms of *reliability* rather than dependability. More specifically, they recommend reliability to be demonstrated in relation to *coding scheme development and application*.

During the *development* of a coding scheme, it is recommended for researchers to adopt an iterative approach that allows for codes to be refined, revised and rejected. Such an approach is likely to increase the consistency with which each code is applied (see *Step 2: Formulating a coding scheme*, Section 5.2.3.1).

During the *application* of the final coding scheme, reliability is commonly demonstrated through one of the following two strategies.

- **Strategy 1:** Having multiple researchers apply the coding scheme to a given portion of the dataset (about 10-20% of the entire dataset is recommended) and calculate a suitable inter-rater reliability (IRR) measure[3]. A high IRR value suggests that reliability may be achieved even if the rest of the dataset is coded by a single researcher. However, if the resulting IRR is moderate to low, it might be more appropriate to opt for Strategy 2.
- **Strategy 2:** Having multiple researchers apply the coding scheme to the entire dataset individually, followed by discussions aimed at identifying discrepancies and resolving *as many of them as possible*. Since this does not imply that *all* discrepancies are resolved, it is important that the researchers report the degree of agreement by providing an IRR measure.

A third strategy (**Strategy 3**) involves returning to the *development* phase. That is, to have multiple researchers code the entire dataset individually, followed by discussions aimed at identifying discrepancies and resolving *all* of

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[3] Cohen’s kappa. Krippendorff’s alpha. Interclass correlation coefficients (ICCs).

them in order to settle for a final coding scheme. Such a strategy is commonly referred to as coding by *negotiated agreement* (Garrison et al., 2006).

5.3.3 Establishing trustworthiness and reliability in my work

Details of the measures taken to ensure trustworthiness and reliability during the data collection and the data analysis have already been outlined in Section 5.2.2.3 and Section 5.2.3.2.

5.4 Ethical considerations

In educational research, aspects of research ethics typically revolve around the multiple responsibilities of the researcher in relation to the research participants, data management, publication and dissemination of results (BERA, 2018). This section outlines the ethical considerations of my research project.

5.4.1 Relationship between researcher and participants

When conducting research that involves the participation of other beings, it is crucial to reflect on your responsibilities as a researcher in relation to your research participants. Within the field of education research, it is especially important to reflect on this matter in situations where the research participants are also your students; in such cases, your responsibilities as their teacher may differ from your responsibilities as a researcher.

For instance, consider that you read about an intervention that has proved effective in increasing students' understanding of the Boltzmann distribution or some other scientific concept. As a researcher, you might feel tempted to divide your group of students in two and thus create a test and a control group to explore said intervention. This would be an appropriate study design. However, as the students' teacher, this would be unfair to the group of students that did not receive the additional support from the intervention (should the intervention prove to be effective). This is a common ethical dilemma for scholars in educational research. You have to be mindful of your role in relation to your research participants and how that might affect the outcome of your research as well as how it might affect your research participants.

It is also important to consider the power (im)balance between you and your students and how that might affect how the students behave during data collection (e.g. interviews or observational studies). This is not only important to consider *during* the data collection but also prior to the data collection itself, during the recruitment of participants. Measures to mitigate any impact from the 'power position' of you as an authoritative figure should be taken (as much as possible).

Me and my research participants did not have a teacher-student relationship during the time that the studies of this thesis were conducted. In the absence of such a power relation, there were no expectations for such structures to influence the choices and/or behaviours of the research participants. It is, however, important to note that I had been teaching the chemistry majors in a course occurring earlier in the semester. Thus, although we did not currently have a teacher-student relationship, the student might have still perceived me as an authoritative figure and experienced a difference in hierarchy.

To mitigate the potential hierarchy gap, I began each interview just sitting down with the students, talking about their courses and their current struggles in- and outside of the academic setting, letting them get to know me and my background before we started. The aim of that conversation was to create a safe space, making sure they understood that I was there merely to explore a research topic of my interest and not to *judge* them or their efforts.

5.4.2 Risks and benefits for participants

Risks. None of my research studies involve any physical interference or bear any risk of harming participants; the risks for participants can be considered minimal. No intentional collection of sensitive data has taken place and should *un*intentional collection of such data take place in the future, it will not be used in the research project. The risk of such an event to occur should, however, be very low as the discussions will be framed by tasks centred around chemical concepts.

Benefits. Both data collections were carried out prior to the students' exams in physical chemistry. Therefore, the problem-solving sessions (during which the data was collected) served as study sessions, providing the students with an opportunity to practice their problem-solving skills in a topic relevant to their exams. Moreover, they had the opportunity to go over the task with the researcher at the end of the problem-solving session.

All research participants received a movie voucher to thank them for their participation. It is important to consider the size of the compensation in relation to recruitment. The participants should not feel as if they have directly or indirectly been *pushed* towards participation. A movie voucher was deemed as a balanced compensation: something the students that could enjoy but that would not be particularly life-changing (depending on the movie).

5.4.3 Recruitment and informed consent

The recruitment process was carried out in two stages.

In the first stage, I visited lectures given at appropriate courses, gave a short oral presentation of the research project (explaining its purpose and how it would be carried out) and handed out a sign-up sheet. Students interested in participating were asked to provide a name and an email address in order for the researcher to be able to distribute more detailed information concerning the study. It was emphasised that entering one's name to the sign-up sheet only meant that one was interested in receiving more information about the study; it did not mean that you consented to participate in the study.

In the second stage, I distributed a formal **Invitation letter** (Appendix II) to all students who signed up, containing more detailed information about the study and providing the students with answers to questions such as: *What will happen during the problem-solving session? How will data be collected, analysed and managed? Can I withdraw from the study? Will I receive any compensation for participating? Who can I contact if I have questions?* The students were given two weeks to review the information and decide whether or not to participate.

The recruitment process outlined above took place *prior* to the data collection. *During* the data collection (i.e. the problem-solving sessions), the students were given another opportunity to read the invitation letter and ask questions before deciding whether or not give written consent by signing a **Consent form** (Appendix III). I made sure that the participants were aware that they had the right to withdraw consent without justification at any point of the research process.

Of the 14 students who showed interest in participating, 12 signed up as pairs. The remaining two signed up individually and were paired up by me after correspondence with the students in question. At the beginning of each problem-solving session, the students were given the opportunity to reconsider their participation before deciding whether or not to give written consent by signing a consent form. All 14 students consented to participate in the study and each of them were compensated with a movie ticket for their participation.

5.4.4 Data collection and analysis

The choice to collect video data came from the anticipation that research participants would point at different parts of a so-called reaction mechanism (sequence of chemical formulas, Appendix I) while discussing the tasks. To avoid collecting 'unnecessary data', the video camera was set up to capture only the students' hand movements.

During the transcription phase, the participants' names were replaced with pseudonyms. The key to these pseudonyms is accessible only to the members of the research team, securely stored in a locked space. To further safeguard the participants' identities, pseudonyms have also been used in various communications of results, including written publications and oral presentations.

5.4.5 Storage of data and GDPR

The collected research data is currently stored in a password-protected storage area on the platform *Dataportal Allvis*, provided and recommended by Uppsala University for the storage of research data. The storage area is shared by the members of the research team and no unauthorised personnel have, or will ever have, access to the research material. Field notes (on paper) and consent forms are kept in a locked space, to which only the members of the research team have access.

In accordance with the guidelines for data retention and deletion of data, the research material will be saved for at least 10 years. All personal data will be treated as strictly confidential as stated by the General Data Protection Regulation (GDPR).

6 Results and discussion

In this chapter, I provide overviews of Paper I and Paper II. Since these two papers offer distinct perspectives on the same set of data, the context and methods used for data collection have already been described in Section 5.2.1 and Section 5.2.2, respectively. This chapter will focus on the specific details pertaining to the analysis, findings, and discussions of each paper.

6.1 Paper I

***How much is just maths?* Investigating problem solving in chemical kinetics at the interface of chemistry and mathematics through the development of an extended mathematical modelling cycle**

Paper I is published in Chemistry Education Research and Practice.

The aim of this paper was to explore the cognitive processes at play during problem solving at the interface of chemistry and mathematics. To this end, we video-recorded problem-solving sessions where student pairs worked with a set of tasks centred around a key concept in chemical kinetics, using think-aloud protocols to follow their reasoning. The video data were transcribed verbatim and analysis of the resulting transcripts was guided by the two research questions below.

- **RQ1:** How can the MMC be refined to provide a framework that allows us to capture and analyse, at a higher level of resolution, the specific processes that students engage in while solving a problem in chemical kinetics?
- **RQ2:** When and how do students use extra-mathematical input during the problem-solving process and what roles do such input play?

6.1.1 Data analysis and findings

A general procedure for the data analyses carried out in my papers, including the measures taken to establish reliability, is given in Section 5.2.3.2. Herein, I provide a more detailed description of the specific analyses carried out to address the research questions of Paper I, including some major findings.

6.1.1.1 Development of the coding scheme: *the extended MMC*

Deductive analysis, employing *the classical mathematical modelling cycle* (MMC, Section 3.3.3) as the initial coding scheme, combined with inductive analysis, resulted in the final coding scheme: *the extended MMC* (Figure 5). In comparison to the classical MMC, our empirically derived analytical framework provides a more fine-grained description of the variety of processes and subprocesses that students engage in during problem solving in chemical kinetics. Additionally, *the extended MMC* offers insight into where in the cycle (during which processes) that students may draw on their *extra-mathematical resources*.

In the following sections, I briefly describe the subprocesses and extra-mathematical resources revealed through data analysis, providing exemplifying quotes where necessary. Note that exemplifying quotes for each code can be found in the corresponding paper (Ye et al., 2024).

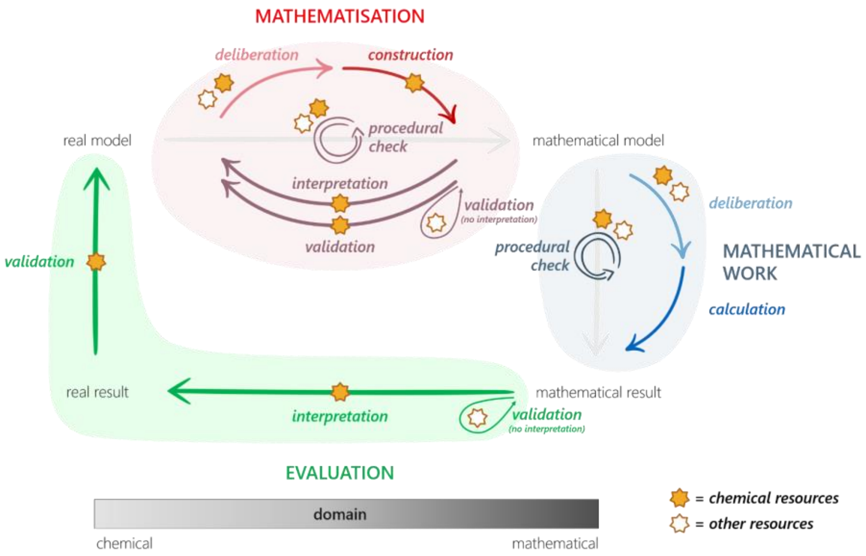


Figure 5. *The extended MMC* captures the processes observed during our data analysis. Each italicised label corresponds to a code and each capital label corresponds to a theme. Codes that belong to the theme mathematisation are illustrated in red and purple, codes that belong to the theme mathematical work are presented in blue tones and codes belonging to the theme evaluation are shown in green. The stars correspond to extra-mathematical resources, with the filled star representing chemical resources and the unfilled star representing *other resources*. A star superimposed on an arrow indicates that the activation of EMRs is inherent to the (sub)process. A star placed next to an arrow indicates that EMRs can be activated as part of that (sub)process. The dichotomy between the real-world and mathematical domains has been replaced with a gradient between a chemical and a mathematical domain, to illustrate the continuous nature of the shift between the two domains observed in our data. Figure reproduced from Ref. Ye et al. (2024).

Subprocesses. An initial round of deductive coding revealed that students engaged in various subprocesses in addition to the processes found in the classical MMC. During the *mathematisation* step, students not only engaged in *model construction,* but also in *deliberation* and *procedural checking.* More specifically, the construction phase included additional subprocesses where students deliberated on how to carry out the model construction and conducted procedural checks to keep track of what they were doing. A similar structure was observed during the *mathematical work*; students not only engaged in technical mathematical calculations but also *deliberated* on how to perform them and carried out *procedural checks* to monitor their work. Interestingly, we found that students evaluated their mathematical models as well as their mathematical results, and that there were *two types of evaluation*: one where the validation of a mathematical result was integrated with interpretation of its physical meaning, and another where the validation occurred without any such interpretation. The difference between these two types of validation is illustrated by the following exchange between Alice and Andrea.

Validation without any interpretation

Andrea: Ok, uhm… Are we supposed to have such a long rate law?

Alice: I don't know… It felt like we were supposed to get something much… Although… Haven't we gotten quite long [rate laws] in like … the tutorials?

Andrea: Hm, yeah, maybe we have? Sometimes you've been able to simplify them heaps… But I… But I don't know, I can't see at all how you could do that here…

Validation with interpretation

Alice: No, but I mean maybe it's kind of reasonable because … it [the formation of oxygen] depends on … this *$C_6H_5CO_3H$, step 2*. It *$C_6H_5CO_3H$, step 1* is the starting material for both the intermediate and then (…) it's part of the last step to form oxygen *step 2*. But I don't know (…) Why would it depend so much on the concentration of this *$C_6H_5CO_3H$*

Andrea: But isn't that because this *$C_6H_5CO_3H$*… I mean this sort of decides how much [of the intermediate] that goes to the backwards-reaction [of the equilibrium step]?'

Alice: Yes, that's right… That's true. Well, in that case it seems kind of reasonable, right?'

Andrea: Yeah, maybe it is… (…)

Alice: It's just … long! [both students laugh]

Extra-mathematical resources. In addition, inductive analysis revealed that students relied on extra-mathematical knowledge (EMK) not only during the domain-bridging processes, as previously suggested, but also during the mathematical work. A closer look at each moment of extra-mathematical input further revealed that EMK did not always correspond to *conceptual chemical knowledge*, as anticipated based on the literature, but included other kinds of 'knowledge' as well. These other kinds of 'knowledge' did not fit well into the categories of mathematical and chemical knowledge; in fact, they did not really fit well into the category of *knowledge* at all. Therefore, we decided to temporarily refer to them as *other resources* and reconceptualised EMK into extra-mathematical *resources* (EMRs). The following quote by Robin is an example of an instance coded as him relying on an *other resource.*

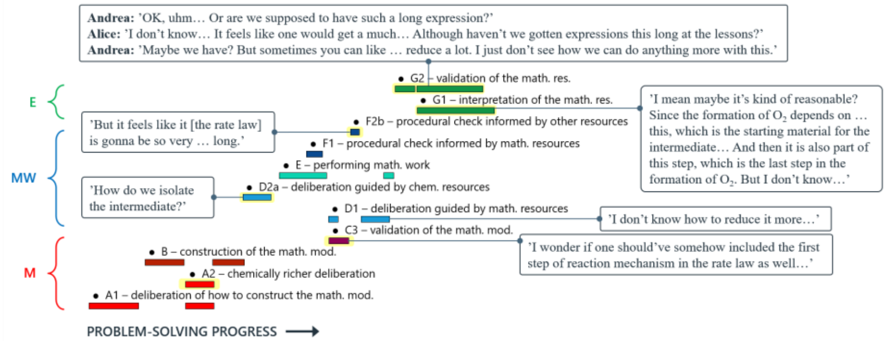
Deliberation of mathematical work guided by other resource

> **Robin:** (…) then we had something about that f**king symmetry that he [the teacher] talked about so that you can just like add them together or something if you feel like it and everything is much easier.

6.1.1.2 Application of the coding scheme: generating problem-solving trajectories to understand 'the bigger picture'

Coded transcripts were also visualised as *problem-solving (PS) trajectories.* Created from the *coding stripes view* in NVivo®, PS trajectories provided us with overview perspectives that turned out to be especially useful for investigating 'the bigger picture' of each problem-solving attempt. Ultimately, analysis of the PS trajectories resulted in five distinct cases, some of which led to further insights into the roles of EMRs. The PS trajectory corresponding to Case 2 is shown in Figure 6.

- **Case 1** illustrated that *technical competence in mathematical manipulations does not suffice* when it comes to problem solving at the interface of chemistry and mathematics; chemical resources can be crucial in guiding the mathematical work towards such success.
- **Case 2** showed that extra-mathematical input (both chemical and *other resources*) can help students stay on track during all stages of the kind of mathematical modelling task investigated in this study.
- **Case 3** showed that extra-mathematical input (both chemical and *other resources*) can help students get back on track.
- **Case 4** indicated that, in some cases, extra-mathematical input can lead students astray.
- **Case 5** illustrated how PS trajectories can be utilised to facilitate the analysis of mathematical modelling data generated by modellers that frequently 'jump' across different stages of the MMC.



Andrea: 'OK, uhm… Or are we supposed to have such a long expression?'
Alice: 'I don't know… It feels like one would get a much… Although haven't we gotten expressions this long at the lessons?'
Andrea: 'Maybe we have? But sometimes you can like … reduce a lot. I just don't see how we can do anything more with this.'

'But it feels like it [the rate law] is gonna be so very … long.'

'How do we isolate the intermediate?'

'I mean maybe it's kind of reasonable? Since the formation of O_2 depends on … this, which is the starting material for the intermediate… And then it is also part of this step, which is the last step in the formation of O_2. But I don't know…'

'I don't know how to reduce it more…'

'I wonder if one should've somehow included the first step of reaction mechanism in the rate law as well…'

Figure 6. PS trajectory of Alice and Andrea's modelling attempt (Case 2). Yellow shadings highlight all instances where they applied EMRs. Quotes have been added to offer a more detailed picture of how they employed their different EMRs. In a PS trajectory, each coded segment of a transcript is plotted with respect to the problem-solving progression. Note that the x-axis does not directly correspond to time; rather, it reflects the relative length (in text) of each coded segment. M: mathematisation; MW: mathematical work; E: evaluation of mathematical result. Figure reproduced from Ref. Ye et al. (2024).

6.1.2 Discussion

This section provides a summary of the findings as they relate to the study's research questions.

6.1.2.1 Enhancing the analytical power of the MMC

RQ1: *How can the MMC be refined to provide a framework that allows us to capture and analyse, at a higher level of resolution, the specific processes that students engage in while solving a problem in chemical kinetics?*

This work contributed to an enhanced resolution of the MMC in two ways: through the identification of subprocesses; and through the visualisation of subprocesses as PS trajectories.

Identification of subprocesses. Data analysis revealed that students engaged in *deliberation* and carried out *procedural checks* during the mathematisation step as well as during the mathematical work. These findings thus suggest that mathematisation goes beyond the mere construction of mathematical models and that mathematical work entails more than technical mathematical manipulations, highlighting the role of metacognitive processes such as planning and reflection during these stages of the MMC.

Deliberation and procedural checks occurred to a higher extent when students seemed unsure of how to proceed and had to engage in decision-making. Tracking these subprocesses may therefore be fruitful in pinpointing *where* in the MMC that modellers struggle the most.

In addition, the observation of students interpreting and validating not only the mathematical result but also the mathematical model, suggests evaluative activities to be essential in all stages of the MMC. This aligns with previous work on validating activity in mathematical modelling (Czocher, 2018).

While none of these observations were particularly unexpected, the increased resolution provided by making the identified subprocesses explicit in the MMC, has important implications for research and practice, contributing to more targeted research efforts and instruction.

Importantly, this is not to imply that the classical MMC lacks in accuracy or robustness. The classical MMC is a *prescriptive* model, recommending what steps a modeler should undertake during mathematical modelling. In contrast, the extended MMC serves as a *descriptive* model, aiming to capture the actual steps undertaken by modelers. Neither of these models is inherently superior or inferior to the other; they simply serve different purposes.

Visualising subprocesses as problem-solving (PS) trajectories revealed a diversity of problem-solving approaches as exemplified by the five cases listed above; some students relied heavily on their mathematical resources and others consistently drew on their extra-mathematical resources (EMRs).

An interesting observation is that students who managed to stay connected to the chemical domain throughout the tasks, were more likely to succeed. Case 3 (Figure 16, in Ye et al. 2024) is a particularly striking example where the students initially relied on their mathematical resources to the point that they got ‘stuck in a loop’, substituting one mathematical expression for another. Eventually, they carried out a procedural check informed by their *other resources*, prompting a sequence of metacognitive actions: they re-evaluated their mathematisation and revised their mathematical model. Ultimately, the EMRs helped the students ‘break the loop and get back on track’.

Although extra-mathematical input seems to benefit this kind of problem solving, it is important to note that simply observing a high frequency of extra-mathematical input does not guarantee task success; it has to be appropriately distributed across the trajectory. For instance, in Case 4 (Figure 17, in Ye et al. 2024), the students relied so heavily on a particular EMR that they overlooked other important information given in the task and were led astray.

Finally, visualising coding as PS trajectories proved particularly useful in analysing complex problem-solving attempts were students frequently jumped across the various stages of the MMC (e.g. form a subprocess in the mathematisation step to one in the mathematical work phase). The power of the PS trajectories in unfolding such problem-solving attempts is illustrated in Figure 6, showing how such bouncing has previously been visualised in the literature and how it may be visualised as a PS trajectory.

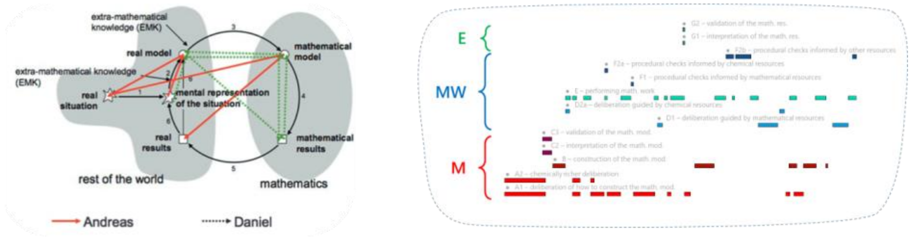


Figure 7. Our visualisation of coded transcripts as problem-solving trajectories facilitates the analysis of modellers' bouncing around in the MMC. Left: Visualisation of how students bounce around in the MMC, reproduced from Ref. Doerr et al. (2017) with permission from Springer Nature. Right: Visualisation of students bouncing around in a problem-solving trajectory view.

6.1.2.2 Exploring EMRs and their roles in mathematical modelling.

RQ2: *When and how do students use extra-mathematical input during the problem-solving process and what roles do such input play?*

In addition to a refinement of the MMC, this work offered valuable insights into the *nature* of extra-mathematical resources (EMRs) and their *roles* during various stages of the MMC.

The nature of EMRs was explored by investigating instances where students relied on resources other than mathematical such. Findings refuted the initial assumption of *extra-mathematical* being synonymous with *chemical*. Rather, EMRs seemed to encompass two distinct classes of resources: *chemical* and *other resources*.

While the former corresponded to students' conceptual understanding of chemical phenomena, the latter consisted of resources that were difficult to categorise as strictly mathematical or chemical. The exchange on page 81, when Alice and Andrea talk about their feelings related to *how long* an expression should be, is an example of an instance that was coded as the students relying on their *other resources*.

Dividing EMRs into these two classes, revealed that the use of chemical resources generally led to more explicit reasoning. When students relied on their chemical resources, they were often able to justify their work by articulating chemical information provided in the task. Conversely, when students relied on their *other resources* they typically expressed themselves in terms of something *feeling* right or wrong. This pointed to the manifestation of some tacit knowledge: a 'gut feeling' of sorts.

Given that reasoning reflecting a reliance on *other resources* may appear less sophisticated and rigorous compared to reasoning grounded in the chemical domain, it might be tempting to dismiss such reasoning as nonsensical and unimportant. However, me and my co-authors argue otherwise, proposing instead that further exploration of instances where students rely on their *other* *resources* could yield valuable insights into the intricacies surrounding the development of intuition.

The roles of EMRs in mathematical modelling were primarily examined through the analysis of students' PS trajectories. While the coding scheme itself revealed during which processes of the MMC that students relied on certain resources, the overview perspective provided by PS trajectories offered insight into the chronological relationship between those processes and other steps in the MMC. In relation to RQ2, the coding scheme answered the question of *when,* whereas the analysis of PS trajectories addressed the question of *how*. Further inquiry into the *when* and *how* of EMRs led to the identification of three roles.

(1) EMRs serve as essential input for *translating* between the chemical and mathematical domain. During the processes of mathematisation and interpretation, input from *chemical resources* are especially important as these are required not only to determine how various chemical phenomena may be described mathematically, but also to interpret the physical meaning of various mathematical values and relationships.

(2) Students rely on EMRs in *defining objectives* to work towards. This reliance was observed both during mathematisation and mathematical work.

(3) Students rely on EMRs to *provide standards* against which evaluation can be performed. This application of EMRs was observed consistently throughout the entire MMC.

As mentioned above, the manifestation of Role 2 and Role 3 depended heavily on which kind of EMR that students relied on. Typically, a reliance on *other resources* would lead to more vague objectives and evaluation standards compared to a use of chemical resources. Borromeo Ferri (2006) has proposed a similar distinction, identifying two types of validation: *knowledge-based* and *intuitive*. Importantly, a *vague* objective or standard for evaluation does not necessarily have to be a bad thing. In this context, 'vague' simply implies that it is less precisely defined, more challenging for the student to articulate, and appears to reflect implicit (tacit) knowledge rather than explicit understanding.

While the literature has acknowledged the importance of EMK (or EMRs) in *certain* stages of the classical MMC, the collective findings of this paper suggests extra-mathematical input to benefit *all* stages of the MMC. This includes the mathematical work, thus challenging the conventional notion of this phase as purely mathematical.

6.1.2.3 Exploring the metacognitive dimensions of the MMC

In addition to the previously mentioned findings, this work paves the way for further exploration into 'the metacognitive dimensions of the MMC' in two significant ways. Firstly, by providing a suitable analytical framework that incorporates metacognitive subprocesses like *deliberation* and *procedural checks*. Secondly, by offering insights into the relationship between procedural checks and other evaluative processes. In many cases, procedural checks seemed to trigger other evaluative processes, thus aligning with the concept of metacognitive 'red flags' introduced by Goos (1998, 2002).

6.2 Paper II (manuscript)

More than numbers and molecules – exploring the nature and roles of non-disciplinary resources during problem solving in chemical kinetics

This paper is a manuscript that has not yet been published.

In Paper I, we defined *other resources* as pieces of knowledge that did not lend themselves to categorisation as either mathematical or chemical, but that students nevertheless relied on during problem solving (Ye et al., 2024). At the time, we did not further specify exactly what these *other resources* were. However, we noted that when relying on *other resources*, students expressed themselves in implicit rather than explicit terms, e.g. referring to whether they *felt* a result to be right or wrong, instead of articulating an underlying chemical mechanism. In this sense, instances where students employed their *other resources* could sometimes appear as them relying on their 'gut feeling' or intuition. This observation, along with the finding that students employed these *other resources* throughout the MMC, sparked an interest in studying them further. Picking up where we had left, the same data as analysed in Paper I was subjected to a few more rounds of analysis, focusing in on the *what* and *why* of *other resources*. The study was guided by the following two questions:

- **RQ1:** How can the nature of *other resources* be characterised in more detail?
- **RQ2:** What roles do *other resources* play during problem solving at the crossroads between chemistry and mathematics?

The conceptual framework employed to explore these questions is similar to that used in Paper I, employing the same methodology and an almost identical theoretical framework. In addition to cognitive science, constructivism, sociocultural theory, the resources framework, and the MMC (our extended version), the theoretical framework employed herein also includes concepts and ideas pertaining to various aspects of general problem solving, such as *metacognition*, *procedural knowledge*, and *intuition.*

6.2.1 Data analysis and findings

A combination of deductive and inductive analysis led to the coding scheme presented in Table 2, offering a refined definition of *other resources* in terms of their *content*. The coding scheme was applied to four transcripts from Paper I. These transcripts were specifically chosen for analysis due to their relatively high frequencies of instances where *other resources* were activated. Visualising the coded transcripts as problem-solving (PS) trajectories provided insight into the *roles* of *other resources* in mathematical modelling.

6.2.1.1 Development of the coding scheme

The development of the coding scheme can be divided into three rounds.

Round 1: Identifying activation of *other resources* and providing context. A first round of deductive analysis was carried out to identify instances where *other resources* were activated and provide these instances with context. With the findings of Paper I indicating that students relied more heavily on their *other resources* in moments of uncertainty, and that *other resources* seemed to trigger metacognitive 'red flags', the initial coding scheme comprised the following three codes.

- Moments where students relied on their *other resources* (code *other resources*). This coding was carried out in line with Ye et al. (2024).
- Moments where students were unsure of how to proceed with the problem solving (code *moment of uncertainty*).
- Moments where metacognitive red flags were triggered (code *red flag triggered*).

Round 2: Exploring the content of *other resources*. Inductive analysis of the *other resources* identified in Round 1, revealed three different categories: *implicit models of results*, *explicit examples from experience*, and *superficial procedural resources*. The latter is exemplified in the following quote.

> **Alice:** I was wondering if we should have included this [reaction] step in our rate law but ... *I just realised that's not how you do it, so this should be OK* [emphasis added].

Here, Alice refers to 'how you do it', thus reflecting a recollection or realisation of what an accepted modelling procedure should be like. Drawing on *the resources framework* (Hammer et al., 2005) and Star's (2005, 2007) reconceptualisation of procedural knowledge, we coded this instance as Alice relying on one of her procedural resources, further specifying it as a *superficial procedural resource*. The choice to code it as superficial was based on the observations that it was not obviously linked to any conceptual understanding (see *Procedural knowledge,* Section 3.2.4) and that Alice did not provide any motivation as to why this would be 'how you do it'.

A deeper exploration of the *superficial procedural resources* revealed two recurring heuristics: the *no intermediates-heuristic,* and the *things might cancel out-heuristic*. While the former refers to the idea that the final expression should not contain any terms involving reactive intermediates, the latter corresponds to the notion that mathematical terms might cancel each other out during the mathematical operations.

Having arrived at a mathematical result, the excerpt below shows Alice and Andrea engaging in evaluating activities. In doing so, they refer to what they are 'supposed to have/get', thus reflecting certain expectations of what a valid result should look like. Two distinct sources of these expectations were identified: *implicit models of results* and *explicit examples from experiences.*

Andrea: Ok, uhm… Or are we supposed to have such a long expression?

Alice: I don't know… It felt like we were supposed to get something much… *But then again, haven't we got kind of long expressions in like ... the tutorials?* [emphasis added]

Andrea: Yeah, maybe we have? Sometimes you've been able to simplify them heaps… But I… But I don't know, I can't see at all how you could do that [reduce the expression] here…

Alice and Andrea initially express themselves rather vaguely, referring to the obtained mathematical expression as *feeling* somewhat off, without specifying the root of this feeling. In other words, the source of their expectations seems to be their 'gut feelings' or intuition. Defining intuition in accordance with Brady et al. 2022 (see also p. 59 in this thesis), i.e. as the manifestation of an individual's tacit knowledge, we coded instances like this as activations of *implicit (tacit) models of results*.

In contrast, Alice's mention of having seen similar results 'in like… the tutorials' (italicised part of the excerpt), reflects a more explicit source of expectations that seemingly builds on analogous examples encountered in earlier instructional situations. We coded instances like this as activations of *explicit examples from experiences*.

Round 3: Separating *other resources* from their *activation pathways*. Inductive analysis further revealed that *implicit models of results* and *explicit examples from experience* were frequently activated through one of the two memory retrieval processes: *recall* or *recognition*. Both recall and recognition are cognitive processes involving the retrieval of information from long-term memory (LTM).

- **Recall** is the ability to remember things by searching for information in LTM. Searches prompted by external cues are referred to as *cued* recall, while 'self-initiated' searches (not prompted by external cues) are referred to as *free* recall (Eysenck & Keane, 2020).

- **Recognition** is the ability to identify an external object as something you have previously encountered. It is always triggered by an external cue, leading to a comparison where the external object is assessed with respect to LTM. The comparison may lead to recognition or lack of thereof (Eysenck & Keane, 2020).

In this work, we observed recall and recognition *cued* by various components of the tasks. With the terminology of the resources framework, both recall and recognition can be described as memory retrieval processes prompted by an individual's *framing* of a task (Section 3.1.4).

Table 2. Adapted coding scheme of Paper II. For the full table, including examples of each code, please visit the original manuscript at the end of this thesis.

CODE	DESCRIPTION
Round 1: Contextual codes	
Moments of uncertainty	Students make a pause in their problem-solving attempt, often discussing how to proceed.
Red flag triggered	Students are bothered by something, e.g. lack of progress, anomalous result or error detection.
Round 2: Other resources	
Implicit model of results	Students articulating their expectations of the result, leading to comparisons between obtained model/result and some expected implicit model of the result.
Explicit examples from experience	Students referring to something that the teacher said or something they have seen in class.
Superficial procedural resources	Students talking about procedure without substantive connections to chemical concepts or the reaction mechanism.
Round 3: Activation pathways	
Recall	Students searching for specific rules or problem-solving approaches in their LTM.
Recognition	Students comparing a model, result, or approach (external objects) with previously encountered examples (internal, often implicit, objects). The result of the comparison can be recognition or lack thereof.

6.2.1.2 Analysis of problem-solving trajectories

Problem-solving (PS) trajectories were generated using the same method as in Paper I. Offering an overview perspective, thus facilitating analysis of events taking place prior and subsequent to a specific instance, renders PS trajectories particularly suitable for visualising the relationships between *other resources* and other kinds of resources.

Analysis of these relationships indicate that: (1) heuristics can contribute with clear problem-solving strategies but can also lead to strategic inflexibility; (2) implicit models can help students navigate by directing their attention, especially in problem solving of familiar tasks; and (3) even unstructured attempts at recall can be productive. These findings are further explored in the discussion that follows (Section 6.2.2.2).

6.2.2 Findings and discussion

This section offers a discussion of the findings as they pertain to the research questions of Paper II.

6.2.2.1 Exploring the *nature* of *other resources*

RQ1: *How can the nature of other resources be characterised in more detail?*

Deductive and inductive analyses led to the identification of three subcategories falling under the broader category of *other resources*: *implicit models of results, explicit examples from experience,* and *superficial procedural resources*. For clarity and ease of reading, I will subsequently refer to the first two subcategories as *implicit models* and *explicit examples*.

Implicit models and explicit examples were observed to influence students' expectations and anticipations during problem solving. When students relied on their implicit models, they typically expressed themselves in terms of how they felt about their work. Conversely, when relying on explicit examples, students would often articulate specific instructional situations.

While the initial coding scheme did not separate activated resources from the manner in which they were activated (and instead contained codes such as *recognition of implicit model* or *recall of explicit example*), we later found it useful to differentiate between the two. For instance, such division made it possible to describe Andrea's question, 'Are we supposed to have such a long expression?' as a lack of recognition arising from a comparison between the obtained result and an implicit model of the expected result. Similarly, Alice's question, 'Haven't we got kind of long expressions in like the tutorials?' could be classified as a recognition of an explicit example.

Ultimately, this separation highlights that, for a problem solver to achieve task success, possessing resources alone is insufficient, various ways to access the relevant resources is also necessary.

Superficial procedural resources were found to encompass two recurring heuristics: the *no intermediates-heuristic,* and the *things might cancel out-heuristic*. Importantly, the heuristics and procedural resources categorised as superficial, were labelled so due to the algorithmic manner in which students *applied* them. Such view of depth and superficiality aligns with that of Star (2007), whose definitions of deep and superficial procedural knowledge are formulated in terms of how problem solvers *use* procedures.

Comparing the problem-solving attempt by David and Diana, with that by Nelly and Noah, illustrates the difference between a deep and superficial use of procedural resources.

Initially, the two groups exhibited identical trajectories: a heavy reliance on the *no intermediates*- and the *things might cancel out-heuristics*, along with an incorrect identification of too many molecular species as relevant intermediates in the given reaction, kept them in endless loops of substituting one mathematical expression for another. The lack of progress eventually triggered metacognitive red flags in both groups. However, while these red flags appeared to assist Nelly and Noah in leveraging resources to break free from the loop, no such breakthrough was observed with David and Diana. Why did one group succeed with the task while the other did not? After all, they seemed to rely on the exact same resources.

To explain this observation, we proposed *a continuum view* of the relationship between procedural and conceptual resources (Figure 8). With this view, a plausible explanation for Nelly and Noah's success would be that their procedural resources were situated on the left side of the continuum. Thus, when alerted by the metacognitive red flag, they could access the corresponding conceptual resources, assess their work, and adjust their strategy accordingly. In contrast, David and Diana's procedural resources may have resided on the right side of the continuum, leading to difficulties in engaging their conceptual resources altogether.

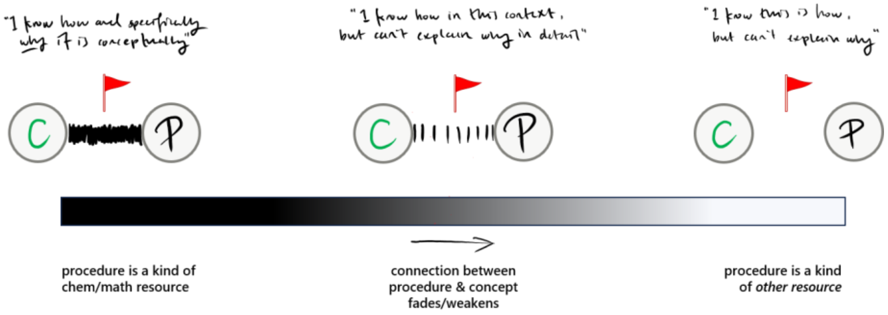


Figure 8. A preliminary model of the interaction between conceptual resources, procedural resources and metacognitive triggers.

Relating this model to the work by Star (2005, 2007), procedural resources that are strongly coupled to conceptual resources should foster a higher level of *flexibility*: a trait of students possessing deep procedural knowledge. Such flexibility has also been reported as a trait of stronger problem-solving skills in general (Jonassen, 2000).

Importantly, we do not assert this as a definitive underlying mechanism of our observation. However, we believe it might be a useful preliminary model of the interaction between procedural resources, conceptual resources and metacognitive red flags, emphasising a continuum rather than dualistic view.

6.2.2.2 Exploring the *roles* of *other resources*

RQ2: *What roles do other resources play during problem solving at the crossroads between chemistry and mathematics?*

Exploring the *roles* of *other resources* through analysis of students' PS trajectories led to three major findings. Before delving into deeper discussions of these findings, I would like to make two clarifications:

(1) While similar to those presented in Paper I, these trajectories feature both the coding stripes that resulted from the current analysis and the coding stripes from Paper 1. The latter has been included to provide readers with insight into the students' locations within the MMC as they use various *other resources*.

(2) Since the code *moments of uncertainty* often span whole sequences of other codes, they are marked as grey boxes/shades in the trajectories only when they provided additional insight for the discussions.

Finding 1: Heuristics can provide clear strategies for problem solving but can also lead to strategic inflexibility. Analysis of David and Diana's PS trajectory showed that they relied primarily on mathematical resources and superficial procedural resources. The combination of the *no intermediates-heuristic* and the students having incorrectly identified too many intermediates as relevant in the given reaction, got them 'stuck in a loop' of substituting one mathematical expression for another. On a few occasions, this lack of progression triggered metacognitive red flags. In those situations, the *things might cancel out-heuristic* typically encouraged the students to persevere with their current approach, hence keeping them in the loop. As such, the two heuristics played distinct roles:

- with the *no intermediates-heuristic* acting as a goal, providing the students with direction during the mathematisation as well as during the mathematical work;
- and the *things might cancel out-heuristic* serving as a motivator, especially whenever doubts arose due to the growing complexity of the mathematical work.

This whole event could be described as a case of *metacognitive failure*: even if David and Diana were able to identify metacognitive red flags, they were unable to adequately address them. Possibly, their strong reliance on the heuristics overshadowed other valuable resources, preventing them from taking a step back and reflect on their approach, essentially limiting their flexibility.

Finding 2: Implicit models and explicit examples can contribute to metacognitive success. Contrary to the example above, the subsequent two cases show how *implicit models* and *explicit examples* can be leveraged to attain *metacognitive success.*

Starting with the case of Nelly and Noah, these students initially found themselves stuck in the same kind of loop as David and Diana. However, in addition to merely noticing that something was wrong (as was the case with David and Diana), Nelly and Noah identified a potential source of the issue: that, perhaps, they had ‘overcomplicated stuff’. Despite its vagueness, this notion seemingly acted as a small beacon, illuminating a path forward.

The following exchange shows how a lack of recognition between their current mathematical result and their implicit models gave rise to metacognitive red flags, and how they eventually addressed these by tapping into their chemical conceptual resources, thus leading to metacognitive success.

Nelly: This was a very complicated rate law *laughs* or are we making it too complicated…?

Noah: Mm… *continues with the mathematical work* Okay, so… Now we still have to add more…

Nelly: Yeah, it’s so much. Won’t this (…) it feels like we’re gon-na get a super long loop… That we’re just adding stuff we need to… substitute! [metacognitive RF triggered]

Noah: Yeah, but now (…) where is the last intermediate (…) which ones do we have to get rid of?

Nelly: This, this, this and that… (…) And in this [term] we’ve got the proton… We’re just adding new intermediates… *laughs*

Noah: Arghhh… did we over complicate stuff somewhere? [met-acognitive RF triggered]

Nelly: (…) It could also be that we, from the beginning, chose too many intermediates (…)

Noah: It’s like you say, if we just look… with respect to the reac-tion…

Nelly: Then the only intermediate… Actually, the proton is not part of this reaction so this [the perbenzoate] is our only intermediate.

The case of Alice and Andrea illustrates instead how activation of an *explicit example* can lead to metacognitive success. While Alice and Andrea managed to avoid ‘the loop’, the length of their obtained mathematical result nevertheless raised a metacognitive red flag. Similar to the case of Nelly and Noah, this red flag resulted from a lack of recognition between their obtained result and their implicit model of what a result should look like in the given context. However, in this case, the red flag corresponded to *metacognitive mirage*: there was actually nothing wrong with their result (Goos, 1998, 2002).

Interestingly, the red flag was ultimately dispelled by an *explicit example*, namely their previous exposure to similarly ‘long’ (or complex) rate laws in tutorials and classes.

The following excerpt shows how a lack of recognition initially triggered a red flag, eventually leading to the recall of an explicit example (italicised in the excerpt below). Seemingly, the explicit example served to broaden the implicit model such that it would encompass also more complex (longer) rate laws. In this way, the explicit example somehow turned the lack of recognition into recognition. Additionally, it appears as if the explicit example provided the students with reassurance, which encouraged them to persist with their approach, and engage in more detailed evaluation of their result, connecting their mathematical result to the chemical information provided by the reaction mechanism.

Alice: (…) It just feels like it's gonna be so very long? [metacognitive RF triggered]

Andrea: Yeah… (…) But I don't know how to simplify it more…

students keep performing mathematical work

Andrea: Ok, uhm… Are we supposed to have such a long rate law?

Alice: I don't know… It felt like we were supposed to get something much… Although… *Haven't we gotten quite long [rate laws] in like … the tutorials?*

Andrea: Hm, yeah, maybe we have? Sometimes you've been able to simplify them heaps… But I… But I don't know, I can't see at all how you could do that here…

Alice: (…) Maybe it makes sense because it [the oxygen production] depends on the starting material of the intermediate, which is also part of this step, I mean the last step to form oxygen, but I don't know…

In summary, implicit models and explicit examples play important roles in troubleshooting and decision-making. While implicit models of results serve primarily as *goals* in these endeavours, explicit examples offer both *goals* and potential *strategies*.

Notably, analysis of our data suggests it is more common for potential issues to be identified through the recognition of implicit models (or rather, lack thereof). However, it seems reasonable that such troubleshooting could also be informed by explicit examples.

Finding 3: Unstructured attempts at recall can be productive and is akin to expert behaviour. While the previous cases mostly involved examples of *other resources* being activated through recognition, the case of Robin and Rebecca was dominated by *recall of explicit examples*. Note that the following three quotes appeared at separate places in the transcript and that all instances of recall were initiated by Robin.

Quotes that illustrate 'recall of explicit examples'

Robin: And then we had that f***ing symmetry that he talked about. That you can like add them together if you feel like it and things get much easier…

Robin: We also have like (…) the equilibrium constant. There was something like that you could do as well…

Robin: But I'm thinking… There was something you could do that you always forget but then you're just like *'Ah, right. That's what you could do…'*

Although these instances of recall were vague in the sense that they did not involve the retrieval of any comprehensive and/or well-defined procedures, the students clearly made use of their recall to navigate the problem-solving activity and explore potential pathways forward. Furthermore, even if this approach might have appeared superficial and random, it actually resembles how experts approach unfamiliar problems: through the application of previously gained knowledge in novel contexts.

7 Conclusions, implications for teaching, limitations and future directions

This chapter begins with an overview of the conclusions derived from the collective findings of my two papers, highlighting their implications for teaching. Subsequently, I address the limitations of my research, acknowledging boundaries and potential areas for refinement. The chapter concludes with a brief introduction to ongoing research and potential avenues for future exploration.

7.1 Conclusions

Solving problems at the crossroads between chemistry and mathematics poses significant challenges for students across all levels of education. Despite the common lament from teachers that ‘students just can’t do maths’, there is now ample evidence suggesting the issue to be rather more complex. With the aim of untangling some of that complexity, this licentiate thesis has focused on the exploration of problem solving in chemical kinetics – a context which requires the integration of knowledge in chemistry and mathematics.

The first step of this inquiry involved the development of an analytical framework suitable for the in-depth analysis of problem-solving activities with both a chemical and a mathematical dimension (Ye et al., 2024). To this end, video data was collected during problem-solving sessions where students worked together in pairs to solve a set of tasks centred around a key concept in chemical kinetics referred to as the steady-state approximation. The video data was transcribed and the resulting transcripts were subjected to deductive and inductive analysis.

Taking inspiration from prior efforts in mathematics and physics education research, Paper I employed an initial theoretical framework combining elements from *the mathematical modelling cycle* (MMC; Borromeo Ferri, 2006) and *the resources framework* (Hammer et al., 2005), thus allowing for the exploration of problem solving in terms of the *processes* that students engaged in and the various *resources* they relied on. Several iterations of deductive and inductive coding yielded *the extended MMC* (Figure 5, p. 80).

Problem solving in chemical kinetics benefits from a closer interaction and coordination between mathematical and chemical resources, with the latter offering guidance to the mathematical operations and providing students with a wider set of problem-solving strategies. The extended MMC suggests that students make use of *extra-mathematical resources* (EMRs) in all stages of the MMC: not only during pre-mathematical activities and mathematisation, as indicated in the existing literature (Niss & Blum, 2020b), but also during mathematical work. Importantly, this does not imply that the activation of EMRs is mandatory in every step of the MMC. However, the findings of this thesis propose that students who do draw on their EMRs throughout the entire modelling procedure are more likely to succeed.

The cases presented in Paper I (Section 6.1.1.2) provide compelling examples, highlighting that proficiency in technical mathematics alone does not guarantee success in problem solving at the crossroads between chemistry and mathematics (Case 1), and emphasising the role of EMRs in goal setting, and troubleshooting (Cases 2 and 3). On this note, analysis of Case 3 further illustrates the distinct roles played by chemical and *other resources*. While *other resources* proved instrumental in alerting the students that something was amiss, chemical resources equipped students with the actual means to revise their strategy, ultimately leading to task success.

Altogether, these findings indicate that problem solving at the crossroads between chemistry and mathematics should benefit from approaches in which each mathematical operation is closely connected to the chemical domain.

Metacognitive activities play a crucial role in the regulation of students' problem-solving strategies, and are reflected in the interactions between students' extra-mathematical resources (EMRs) and the subprocesses of the extended MMC. The extended MMC indicates that students engage in various *(sub)processes* beyond those traditionally outlined in the classical MMC. For instance, during the processes of mathematisation and mathematical work, students not only construct mathematical models and perform calculations; they also engage in *deliberations* on how to construct and calculate, and undertake *procedural checks* to ensure the accuracy of their constructions and calculations. Furthermore, the extended MMC asserts that students may engage in *interpretation* and *validation* not only of their mathematical results but also of their mathematical models.

Adding to this, analysis of problem-solving (PS) trajectories proved useful in examining the interactions between these subprocesses and EMRs, showing that students leverage their EMRs to: (1) formulate goals providing guidance in their deliberations; (2) establish reference points for procedural checks; and (3) setting standards for validation. Interestingly, these interactions seem to reflect metacognitive activities such as planning, monitoring, and validating one's own thoughts and actions.

It is worth noting that chemical and *other resources* play slightly different roles during these metacognitive undertakings. Chemical resources provide students with explicit content regarding the goals, references, and standards. While *other resources* serve these purposes as well, albeit in a more implicit manner, they primarily aid students in identifying issues by triggering metacognitive 'red flags' (see *Goos's metacognitive pathways*, Section 3.2.5.2). These metacognitive red flags can initiate sequences of metacognitive actions, prompting students to pause, engage in procedural checks, and potentially revise their problem-solving approach.

Collectively, these findings underscore the significance of metacognitive activities in regulating students problem-solving approaches, and demonstrate that these metacognitive activities can be captured through the interactions between students' EMRs and the subprocesses of the extended MMC.

There are various *other resources*, beyond chemical and mathematical, that influence students' intuitive decision-making during problem solving in chemical kinetics. Findings from Paper II suggest that *other resources* can be divided into three subgroups: implicit models of results, explicit examples from experience, and superficial procedural resources. Combining this finer-grained characterisation of *other resources* with analysis of PS trajectories reveals that implicit models of results primarily influence students' ideas of *where they are going*, while explicit examples from experience and superficial procedural resources serve instead as a basis of strategies for *how to get there*.

Notably, when students relied on this group of resources, they typically expressed themselves in terms of whether a result *felt* right or wrong, and whether they were *supposed to* do this or that, without articulating the specific reasons behind those feelings and actions. This observation suggests that there is a relationship between *other resources* and *tacit knowledge*, i.e. a kind of 'silent' knowledge that is difficult to put into words but that still shapes an individual's actions and behaviours.

Considering that tacit knowledge is inherently challenging to articulate and make explicit, it is reasonable to assume that it operates in the subconscious – beyond a problem solver's conscious control. If *other resources* function in a similar manner, this implies that they will influence how students approach a given problem, regardless of the students' own intentions. Hence, even though a reliance on *other resources* may appear as haphazard and less sophisticated compared to a reliance on chemical resources, I argue that instances where students rely on *other resources* have educational value and merit scholarly attention. After all, these *other resources* will inevitably impact our students' problem-solving behaviours. For this reason, we should acknowledge the role of *other resources* in problem solving and investigate how they may be leveraged effectively, rather than dismissing them as unimportant nonsense.

Although there is still much to explore, these findings suggest that students' decision-making in problem-solving activities at the interface of chemistry and mathematics is influenced not only by chemical and mathematical resources, but also by non-disciplinary *other resources* that offer guidance on *where to go* and *how to get there*.

7.2 Implications for teaching

The ultimate goal of chemistry education research (CER) is to enhance chemistry education. This includes improving students' learning experiences and outcomes, providing teachers with opportunities for professional development, aiding policymakers in making informed decision, and much more. To ensure that all these stakeholders can benefit from research, it is imperative for chemistry education researchers to translate their findings into recommendations that can be put into action in real-world educational settings. As such, scholarly works in CER often include a dedicated section on the *implications for teaching* that aims to bridge the gap between theory and practice.

In this section, I outline the implications of my research findings for the teaching and learning of chemical kinetics.

The increased resolution of the extended MMC contributes with a richer foundation for targeted instruction. Compared to the classical MMC, the extended MMC provides a finer-grained picture of the processes at play, and the resources employed by students, during problem solving at the crossroads between chemistry and mathematics. This increased resolution comes with two key implications for teaching. Firstly, by making the subprocesses explicit in the MMC, we are now able to pinpoint, with better precision, *where* in the cycle (i.e. during which steps of the MMC) that students encounter challenges. Secondly, the added entry points of input from extra-mathematical resources (EMRs), including chemical and *other resources*, gives us a better idea of what factors that come into play as students attempt to resolve those challenges. Altogether, this increased resolution, in combination with the introduction of the problem-solving (PS) trajectories, greatly enhances the analytical power of the MMC, enabling us to provide targeted instruction with higher precision.

There is a need for more teaching and learning through problem-solving activities that are rich in the use and coordination of both mathematical and extra-mathematical resources. My research suggests that students who maintain a connection to the chemical domain in all stages of the MMC, including the mathematical work, are more likely to achieve task success. Although isolated mathematical *calculations* (e.g. the multiplication of two factors or the addition of two terms) can be performed without guidance from chemical resources, EMRs are crucial during *deliberation* and in *procedural* *checks*. In these subprocesses, both chemical and *other resources* influence students' ideas of where they are and should be heading.

These findings highlight the importance of teaching mathematics not only through context-free mathematical drills that focus primarily on transmitting technical mathematical skills, but also through alternative methods that shed light on the structural role of mathematics. In this regard, I encourage teachers in chemistry and mathematics to:

- teach mathematics through methods that place greater emphasis on the conceptual understanding of mathematics;
- avoid framing mathematics in chemistry as 'just maths' and, instead, be more explicit about the mathematical formalisms that underlie the descriptions of chemical phenomena
- use problems that are rich in contextual factors, prompting students to draw both their mathematical and extra-mathematical resources

While this list is by no means exhaustive, it offers some guidance on how we may create learning opportunities that allow for our students to hone the connections between various resources and, in that way, help them develop a deeper appreciation of the relationship between chemistry and mathematics.

In order to foster the habit of evaluating, educators should strive to design learning materials that incorporate prompts that encourage students to engage in, and reflect on, various types of evaluation. This licentiate thesis contributes with three major findings related to evaluation in mathematical modelling. Firstly, continuous evaluation is crucial for effective mathematical modelling. Secondly, two types of validation exist: *validation with interpretation*, where students activate their chemical resources to make sense of mathematical models and results; and *validation without any interpretation*, where students compare their mathematical models and results with respect to their *other resources*. Thirdly, students generally lack the habit of evaluating their mathematical models/results, and when they do, they tend to skip interpretation and go straight for validation (i.e. they are more likely to engage in validation without any interpretation).

Collectively, these findings advise teachers to: (1) help students realise the importance of evaluating their work throughout the modelling procedure; and (2) provide students with opportunities to practice their evaluative skills.

Recommended learning activities include engaging students in discussions about various *types* of validation (i.e. with and without interpretation). Such discussions should also cover in which situations it might be more appropriate to employ on type of validation than the other, and vice versa. Furthermore, to help students develop a habit of interpreting and validating their work, it is advisable for teachers to include explicit prompts about these steps in various learning material. Importantly, in order to prevent students from developing a dependency on pre-defined prompts, it is essential to gradually decrease the frequency of such prompts as students progress in their learning.

Encouraging students to engage in deliberations and procedural checks can help promote the development of metacognitive skills. Metacognition essentially means *to think about one's own thinking*; engaging in *deliberations* and *procedural checks* may therefore be considered as metacognitive actions. In order to encourage students to deliberate on their work, carry out procedural checks, and thereby foster the development of metacognitive skills, I advise practitioners to create opportunities that allow for collaborative learning. This recommendation is grounded in the belief that my research design, employing *a think-aloud protocol* to follow students as they worked together in *pairs*, likely influenced the prevalence of explicit deliberation and procedural checks in my data.

Making students aware of the covert factors that may influence how they approach a problem, should provide them with better tools for navigating decision-making. While metacognitive actions are inherently *conscious*, the findings of this thesis suggest there are *subconscious* aspects of problem solving that may also impact task success. For instance, various pieces of students' tacit knowledge, including their implicit models of results, are likely to shape how they frame, and ultimately approach, a task.

Moreover, *other resources* can act as triggers of metacognitive 'red flags.' For instance, a lack of recognition between an obtained result and a student's implicit models of results, can give rise to a metacognitive red flag, prompting further deliberation and/or evaluation.

Although these subconscious processes and tacit pieces of knowledge are, by definition, challenging to discern and access, just making students aware of the fact that their problem-solving approaches may be influenced by overt *as well as* covert factors, has the potential to provide them with slightly more navigational clarity and enhance their decision-making skills.

7.3 Limitations

As a step in enhancing the trustworthiness of this thesis, I herein acknowledge some limitations to its claims.

Limitations of the task design. Firstly, my task design did not require students to engage in all stages of the MMC. Rather than having them develop a real model from experimental data, students were provided with a *real model* (i.e. the reaction mechanism) at the outset of the problem-solving session. While this means that none of my studies have investigated what Niss and Blum (2020b) refer to as *full-fledged* mathematical modelling, I argue that such an approach was necessary in this initial phase of my inquiry. Secondly, students were familiar with the type of task employed in the data collection (i.e. the derivation of rate laws from a given reaction mechanism). On the one hand, this familiarity might have prompted students to approach the task algorithmically. On the other hand, it yielded a fairly structured and manageable dataset. Although this may have limited the capture of instances where students grappled with novel challenges, it proved advantageous at this early stage of my research project, facilitating the development of my analytical framework.

Having established a suitable framework, I am now ready to explore more uncharted territories of mathematical modelling in chemistry. In Section 7.4, I briefly outline an ongoing study that aims to address the above-mentioned limitations by using a set of tasks that is less familiar to the students, requiring them to develop a real model from experimental data without prior exposure to similar examples.

Limitations of the data analyses. One member of the research team behind the work presented in this thesis served as the teacher who taught the module on chemical kinetics in the physical chemistry course from which the research participants were recruited. This teacher-students relationship might have influenced both the students' responses during the data collection, and the researcher's interpretation of the data during data analysis. To address these concerns, another researcher took charge of both the data collection and the initial phases of the data analyses. A more detailed discussion of these measures is given in Section 5.2.3.2.

Limitations of the resources framework. The resources framework enables us to describe the mechanisms that underlie learning as dynamic networks of cognitive units. While I acknowledge the explanatory power afforded by this view, it is important to also recognise that it comes with certain limitations.

A significant challenge associated with the resources framework stems from the ambiguous nature of resources, which can vary considerably in their grain-size. This challenge became particularly evident to me during the data analysis of Paper II, during which I initially considered *recognition of implicit models of results* as corresponding to a single resource, but later concluded that a more accurate characterisation would be to consider it as a combination of both a process and a resource. With no strict definitions governing what qualifies as 'a resource,' either of these characterisations were possible.

This example underscores the challenge of defining resources in a way that ensures consistency and comparability within and across studies: the process of defining resources can be influenced by the study context as well as the qualitative judgements of the researcher. Consequently, researchers should exercise caution to prevent introducing inconsistencies within their own data and carefully consider the conclusions drawn when making comparisons with data analysed by others.

As a final note, I emphasise that practicing transparency is crucial in all research endeavours (especially within the subjectivist tradition), not the least when employing the resources framework.

7.4 Ongoing and future research

In this section I briefly discuss ongoing work as well as some potential ideas for future research.

7.4.1 Ongoing research: delving deeper into *mathematisation*

In line with the literature on the teaching and learning of mathematical modelling (e.g. Jankvist & Niss, 2020; Jensen et al., 2017; Niss, 2017b; Niss & Blum, 2020b), my research findings indicate that students struggle considerably more with *mathematisation* than other steps of the MMC (Ye et al., 2024). Given this evidence, I have decided to conduct a study that delves deeper into how chemistry students undertake *mathematisation* in chemistry. The study is currently guided by the following research questions:

- **RQ1:** What hurdles do students encounter during mathematisation of chemical phenomena?
- **RQ2:** What strategies do students apply to overcome these hurdles?

Similar to my previous studies, data will be gathered through video-recorded problem-solving sessions where students work together in pairs to solve a set of tasks in chemical kinetics, employing think-aloud protocols to capture their reasoning. However, to focus in on the specific processes at play during mathematisation, the tasks will be designed to ensure that the chemical concepts addressed are familiar to the research participants, while the mathematical work involves only basic arithmetic operations. The intention behind such task design is to concentrate the challenges to the mathematisation process by preventing students from 'getting stuck' in other parts of the MMC.

In a pilot study, I provided the research participants with a series of time-resolved absorption spectra and asked them to determine the corresponding reaction order. Adhering to the aforementioned criteria, the chemical concepts addressed in the task were familiar to the students, while the mathematical work necessary to solve the task involved only basic arithmetic operations. The mathematisation, however, required translation of time-dependent spectroscopic data into an appropriate mathematical model – a kind of mathematisation that the students had, most likely, not encountered before.

Preliminary findings confirm that students generally struggle more with the mathematisation than the mathematical work. While none of the student pairs were able to solve the task without any guidance from the researcher, they generally expressed no difficulties in following the solution of the task once it was presented to them. As evident from the quote: ‘The maths was not difficult to grasp, but it is challenging to do it when you hadn’t seen it before’, their struggle did not revolve around how to perform the required mathematical operations. Moreover, the students consistently failed to consider that the optical absorption of the mixture could have contributions from two distinct molecular species, leading to difficulties in selecting the appropriate parameters to mathematise.

Altogether, these observations suggest that, for this kind of task, the challenge lies in deciding which parameters to mathematise, rather than in the actual translation. Importantly, the selection of relevant parameters is a crucial part of *pre-mathematisation.* Our preliminary findings thus agree with the existing literature, which has identified pre-mathematisation as another a particularly challenging step of mathematical modelling (Jankvist & Niss, 2020).

Another interesting observation from this preliminary analysis was that several student pairs expressed uncertainty about *what they were allowed to do or not.* Specifically, they seemed unsure about which mathematical operations were permitted within the given chemical context, frequently referring to various actions as ‘illegal’. This preliminary finding suggests a deeper exploration of students’ *epistemological resources* as a potential avenue for future research.

7.4.2 Future research

Exploring the impact of epistemological resources on students’ problem-solving approaches. While I have already begun to investigate how students rely on their *conceptual* and *procedural* resources during problem solving, I would also like to explore the influence of *epistemological* resources on students’ problem-solving behaviours. To the best of my knowledge, there is currently little to no research on the impact of epistemological resources within the context of problem solving at the interface of chemistry and mathematics. Hence, I am particularly keen to inquire whether epistemological resources are disciplinary in nature, and if so, how students navigate situations requiring them to rely on epistemological resources from different disciplines. While my ongoing study has offered initial insights into this matter within the specific context of problem solving in chemical kinetics, I intend to continue this exploration through a collaborative effort with a colleague in physics education research, expanding the research scope to also consider the processes and resources that influence students’ problem-solving approaches at the interface of physics and mathematics.

Exploring the underlying mechanisms of disciplinary intuition. Another intriguing avenue for future research involves delving into the development of disciplinary intuition. While I am still in the process of figuring out how to best approach this topic, and what questions I would like to explore, these are some preliminary questions that are currently circulating in my mind: From a resources perspective, what kinds of resources serve as the basis for intuition? Where do these come from? And viewing intuition as the manifestation of one's tacit knowledge, can pieces of tacit knowledge be traced back to explicit events? How does an explicit cognitive unit transform into an implicit such? Furthermore, is intuition influenced by disciplinary boundaries? And how do students, and experts, navigate situations where conflicts between different intuitive responses may arise?

Further exploration of the metacognitive dimensions of mathematical modelling. Finally, the heightened resolution offered by the extended MMC opens up new opportunities for exploring the metacognitive dimensions of mathematical modelling. As briefly discussed in Section 7.1, I believe that a more detailed examination of how students employ various EMRs during certain subprocesses, such as deliberations and procedural checks, should yield valuable insights into this matter.

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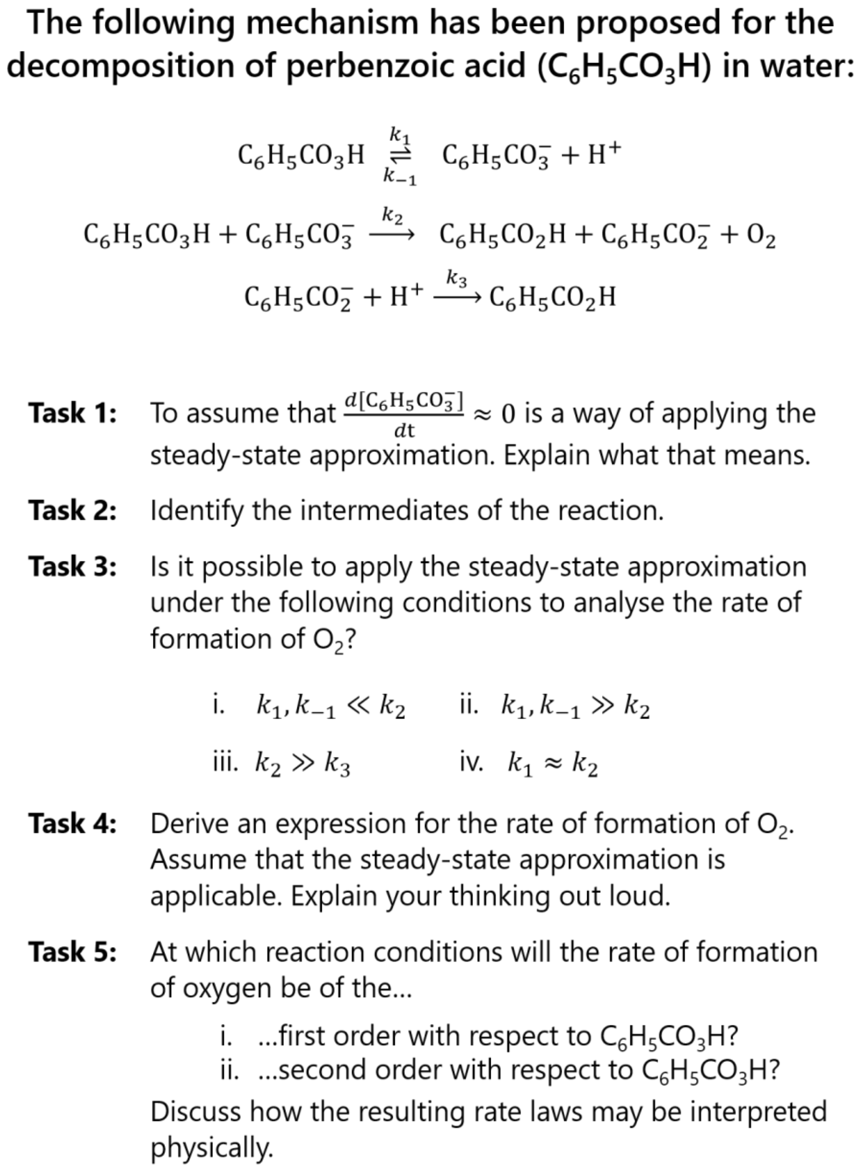
Appendix I: Task 4 and reaction mechanism



The following mechanism has been proposed for the decomposition of perbenzoic acid ($C_6H_5CO_3H$) in water:

$$C_6H_5CO_3H \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_6H_5CO_3^- + H^+$$

$$C_6H_5CO_3H + C_6H_5CO_3^- \xrightarrow{k_2} C_6H_5CO_2H + C_6H_5CO_2^- + O_2$$

$$C_6H_5CO_2^- + H^+ \xrightarrow{k_3} C_6H_5CO_2H$$

Task 1: To assume that $\frac{d[C_6H_5CO_3^-]}{dt} \approx 0$ is a way of applying the steady-state approximation. Explain what that means.

Task 2: Identify the intermediates of the reaction.

Task 3: Is it possible to apply the steady-state approximation under the following conditions to analyse the rate of formation of O_2?

i. $k_1, k_{-1} \ll k_2$ ii. $k_1, k_{-1} \gg k_2$

iii. $k_2 \gg k_3$ iv. $k_1 \approx k_2$

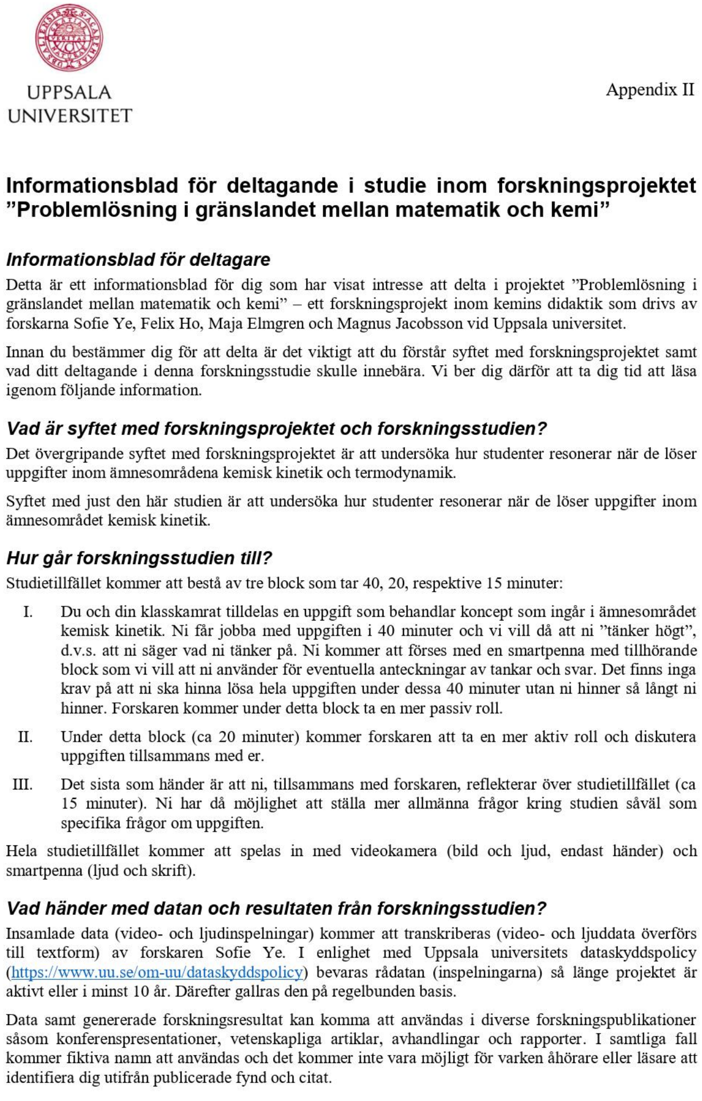
Task 4: Derive an expression for the rate of formation of O_2. Assume that the steady-state approximation is applicable. Explain your thinking out loud.

Task 5: At which reaction conditions will the rate of formation of oxygen be of the...

i. ...first order with respect to $C_6H_5CO_3H$?
ii. ...second order with respect to $C_6H_5CO_3H$?

Discuss how the resulting rate laws may be interpreted physically.

Appendix II: Invitation letter



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Appendix II

Informationsblad för deltagande i studie inom forskningsprojektet ”Problemlösning i gränslandet mellan matematik och kemi”

Informationsblad för deltagare

Detta är ett informationsblad för dig som har visat intresse att delta i projektet ”Problemlösning i gränslandet mellan matematik och kemi” – ett forskningsprojekt inom kemins didaktik som drivs av forskarna Sofie Ye, Felix Ho, Maja Elmgren och Magnus Jacobsson vid Uppsala universitet.

Innan du bestämmer dig för att delta är det viktigt att du förstår syftet med forskningsprojektet samt vad ditt deltagande i denna forskningsstudie skulle innebära. Vi ber dig därför att ta dig tid att läsa igenom följande information.

Vad är syftet med forskningsprojektet och forskningsstudien?

Det övergripande syftet med forskningsprojektet är att undersöka hur studenter resonerar när de löser uppgifter inom ämnesområdena kemisk kinetik och termodynamik.

Syftet med just den här studien är att undersöka hur studenter resonerar när de löser uppgifter inom ämnesområdet kemisk kinetik.

Hur går forskningsstudien till?

Studietillfället kommer att bestå av tre block som tar 40, 20, respektive 15 minuter:

I. Du och din klasskamrat tilldelas en uppgift som behandlar koncept som ingår i ämnesområdet kemisk kinetik. Ni får jobba med uppgiften i 40 minuter och vi vill då att ni ”tänker högt”, d.v.s. att ni säger vad ni tänker på. Ni kommer att förses med en smartpenna med tillhörande block som vi vill att ni använder för eventuella anteckningar av tankar och svar. Det finns inga krav på att ni ska hinna lösa hela uppgiften under dessa 40 minuter utan ni hinner så långt ni hinner. Forskaren kommer under detta block ta en mer passiv roll.

II. Under detta block (ca 20 minuter) kommer forskaren att ta en mer aktiv roll och diskutera uppgiften tillsammans med er.

III. Det sista som händer är att ni, tillsammans med forskaren, reflekterar över studietillfället (ca 15 minuter). Ni har då möjlighet att ställa mer allmänna frågor kring studien såväl som specifika frågor om uppgiften.

Hela studietillfället kommer att spelas in med videokamera (bild och ljud, endast händer) och smartpenna (ljud och skrift).

Vad händer med datan och resultaten från forskningsstudien?

Insamlade data (video- och ljudinspelningar) kommer att transkriberas (video- och ljuddata överförs till textform) av forskaren Sofie Ye. I enlighet med Uppsala universitets dataskyddspolicy (https://www.uu.se/om-uu/dataskyddspolicy) bevaras rådatan (inspelningarna) så länge projektet är aktivt eller i minst 10 år. Därefter gallras den på regelbunden basis.

Data samt genererade forskningsresultat kan komma att användas i diverse forskningspublikationer såsom konferenspresentationer, vetenskapliga artiklar, avhandlingar och rapporter. I samtliga fall kommer fiktiva namn att användas och det kommer inte vara möjligt för varken åhörare eller läsare att identifiera dig utifrån publicerade fynd och citat.

All information som samlas in om dig kommer att hållas konfidentiell och lagras på en lösenordskyddad plattform som tillhandahålls av Uppsala universitet. Ingen obehörig person kommer att ha tillgång till materialet. server som endast behöriga forskare har tillgång till. Ingen obehörig kommer att kunna ta del av inspelningarna eller din medgivandeblankett.

Varför har jag blivit inbjuden att delta?

Du är inbjuden att delta eftersom du deltar i en kurs där kemisk kinetik är en del av innehållet.

Finns det några särskilda risker med att delta?

Det finns inga särskilda risker med att delta i projektet.

Måste jag delta i studien?

Nej – det är helt och hållet upp till dig! Väljer du att delta, bör du behålla detta informationsblad för att visa att du tagit del av, och förstått, vilka rättigheter du har som deltagare i forskningsprojektet. Du behöver också fylla i medgivandeblanketten för att bekräfta att du vill delta.

Vad gäller om jag vill dra mig ur projektet?

Du kan när som helst dra dig ur studien. Du behöver inte uppge någon orsak till att du drar dig ur och det kommer inte att påverka dig eller dina studieresultat.

Om du vill dra dig ur studien ber vi dig att kontakta forskningsledaren, Sofie (sofie.ye@kemi.uu.se), så snart som möjligt efter genomfört deltagande. Utifall att forskningsledaren skulle vara frånvarande kan ni kontakta Felix Ho (felix.ho@kemi.uu.se) så att er förfrågan kan besvaras så snabbt som möjligt.

Kompensation

Som tack för ditt deltagande kommer du att få en biobiljett.

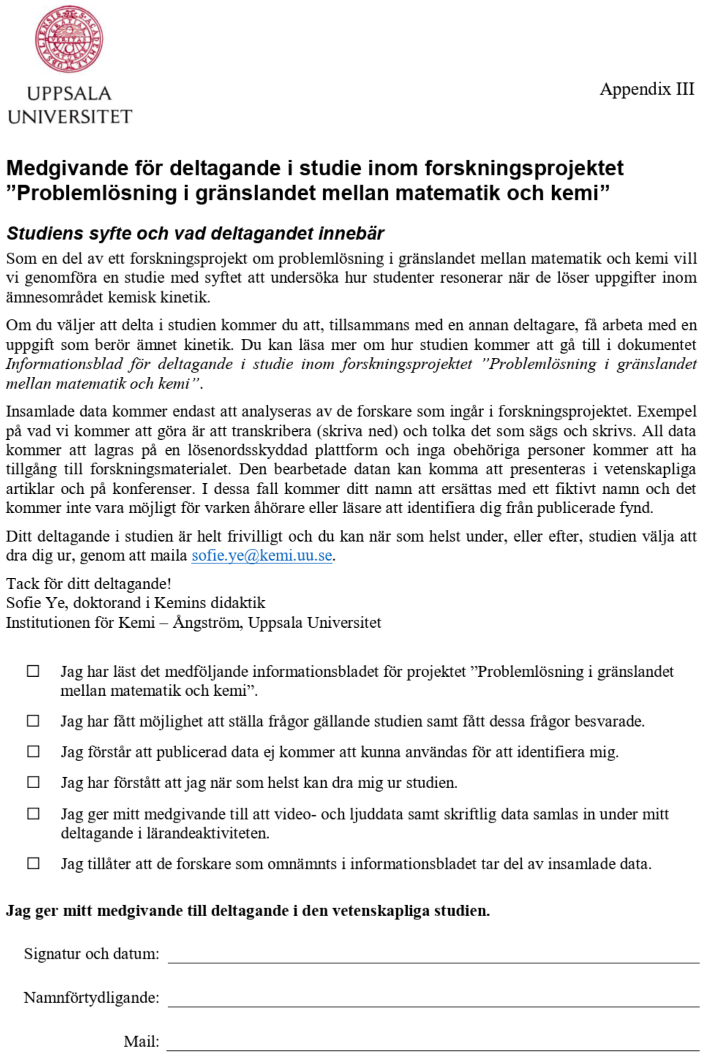
Klagomål

Om du känner dig missnöjd med något i forskningsstudien, börja med att kontakta forskningsledaren Sofie Ye (sofie.ye@kemi.uu.se). Om du fortfarande känner dig missnöjd efter detta och vill lägga ett formellt klagomål, alternativt om du bara vill prata med någon annan, är du välkommen att kontakta forskningsgruppens ledare Johannes Messinger (johannes.messinger@kemi.uu.se) eller Uppsala universitets dataskyddsombud (dataskyddsombud@uu.se). Var i de senare två fallen noga med att specificera forskningsprojektet, namn på forskaren samt vad klagomålet gäller.

Dataskyddspolicy

Som deltagare har du, enligt dataskyddsförordningen, rätt att få svar på om och hur Uppsala universitet behandlar dina personuppgifter (rätten till tillgång). Du har även rätt till att begära rättelse, radering och/eller begränsning av dina personuppgifter. Mer information om Uppsala universitets Dataskyddspolicy och hur vi hanterar personuppgifter hittar du på hemsidan https://www.uu.se/om-uu/dataskyddspolicy.

Appendix III: Consent form



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Appendix III

Medgivande för deltagande i studie inom forskningsprojektet ”Problemlösning i gränslandet mellan matematik och kemi”

Studiens syfte och vad deltagandet innebär

Som en del av ett forskningsprojekt om problemlösning i gränslandet mellan matematik och kemi vill vi genomföra en studie med syftet att undersöka hur studenter resonerar när de löser uppgifter inom ämnesområdet kemisk kinetik.

Om du väljer att delta i studien kommer du att, tillsammans med en annan deltagare, få arbeta med en uppgift som berör ämnet kinetik. Du kan läsa mer om hur studien kommer att gå till i dokumentet *Informationsblad för deltagande i studie inom forskningsprojektet ”Problemlösning i gränslandet mellan matematik och kemi”*.

Insamlade data kommer endast att analyseras av de forskare som ingår i forskningsprojektet. Exempel på vad vi kommer att göra är att transkribera (skriva ned) och tolka det som sägs och skrivs. All data kommer att lagras på en lösenordsskyddad plattform och inga obehöriga personer kommer att ha tillgång till forskningsmaterialet. Den bearbetade datan kan komma att presenteras i vetenskapliga artiklar och på konferenser. I dessa fall kommer ditt namn att ersättas med ett fiktivt namn och det kommer inte vara möjligt för varken åhörare eller läsare att identifiera dig från publicerade fynd.

Ditt deltagande i studien är helt frivilligt och du kan när som helst under, eller efter, studien välja att dra dig ur, genom att maila sofie.ye@kemi.uu.se.

Tack för ditt deltagande!
Sofie Ye, doktorand i Kemins didaktik
Institutionen för Kemi – Ångström, Uppsala Universitet

- ☐ Jag har läst det medföljande informationsbladet för projektet ”Problemlösning i gränslandet mellan matematik och kemi”.
- ☐ Jag har fått möjlighet att ställa frågor gällande studien samt fått dessa frågor besvarade.
- ☐ Jag förstår att publicerad data ej kommer att kunna användas för att identifiera mig.
- ☐ Jag har förstått att jag när som helst kan dra mig ur studien.
- ☐ Jag ger mitt medgivande till att video- och ljuddata samt skriftlig data samlas in under mitt deltagande i lärandeaktiviteten.
- ☐ Jag tillåter att de forskare som omnämnts i informationsbladet tar del av insamlade data.

Jag ger mitt medgivande till deltagande i den vetenskapliga studien.

Signatur och datum: ____________________

Namnförtydligande: ____________________

Mail: ____________________