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## Students' thinking about chemical analysis: an investigation within the conceptual profile theoretical framework

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This work presents the determination of the different ways of thinking about chemical analysis that comprise the zones of a conceptual profile model of this concept. A deductive-inductive qualitative approach was adopted to analyze primary data obtained from secondary school and university students' responses to interviews related to chemical analysis. The previously suggested expanded categories of ways of thinking about chemical analysis that emerged from the study of historical and epistemological sources (sociocultural domain) as well as students' alternative ideas (ontogenetic domain) were utilized as a coding framework for the analysis of primary data obtained from students' responses (microgenetic domain). Following dialogic interaction among all three data sources, six conceptual profile zones were established: everyday analysis, alchemical analysis, empirical analysis, compositional analysis, mechanistic analysis and automated analysis.

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### Introduction

According to Sevian and Talanquer (2014), chemical thinking is defined as “the development and application of chemical knowledge and practices with the main intent of analyzing, synthesizing and transforming matter for practical purposes”. The wide variety in students' perceptions and ways of thinking about many chemical concepts (Talanquer, 2013; Yan and Talanquer, 2015; Cooper *et al.*, 2016; Moon *et al.*, 2017; Caspari *et al.*, 2018) pose major challenges in chemistry education.

The conceptual profile framework was proposed by Mortimer and his colleagues (2012) to emphasize the diversity of students' thinking. A conceptual profile model consists of the zones that represent different ways of thinking about a concept. Each zone is defined, established and stabilized by ontological, epistemological and axiological commitments about its meaning (Mortimer *et al.*, 2014a). The conceptual profile framework is a tool that helps students expand their thinking by embracing new scientific concepts and teachers uncover the many ways themselves and their students think and talk in science classrooms (Mortimer *et al.*, 2012, 2014a; Orduña Picón *et al.*, 2020; da Silva Costa and dos Santos, 2022).

Determining the zones of conceptual profile models of ontoconcepts (broad categories related to key fundamental concepts of contemporary science, such as matter, energy and life) was the original goal of the conceptual profile research program. Subsequently, as the research program expanded, these ontoconcepts progressively shifted to more specific concepts (El-Hani *et al.*, 2023). Some examples are the following: life (concept of life, death, living organisms and adaptation) (Mortimer *et al.*, 2012; Coutinho *et al.*, 2014; Nicolli and Mortimer, 2014; Sepulveda *et al.*, 2014), nature (Lönn *et al.*, 2016), time (Sodre and Mattos, 2022), thermal physics (Aguiar, 2014) and more specifically heat, entropy, spontaneity (do Amaral *et al.*, 2014) and energy (Aguiar *et al.*, 2018), matter (particle models of matter, atoms, atomic theories, molecules, substances) (Mortimer *et al.*, 2012; do Amaral *et al.*, 2018; Orduña Picón *et al.*, 2020; Fauziah and Novita, 2022; Pereira and Mortimer, 2025), chemical bonding (Baltieri *et al.*, 2021), chemical reactions (Solsona *et al.*, 2003), equilibrium (da Silva Costa and dos Santos, 2022) and chemistry as a distinct scientific field (Freire *et al.*, 2019).

Building a conceptual profile for the concept of chemical analysis is crucial because it is a fundamental and indispensable component of chemistry (Hudson, 1992; Karayannis and Efstathiou, 2012) both as a system of knowledge as well as a professional field (Vershinin and Zolotov, 2009). Specifically, chemical analysis includes both material entities (the targets and/or endpoints of analysis) and analytical procedures (Chi *et al.*, 1994; Klein and Ragland, 2014; Sevian and Talanquer, 2014) and, among other things, it is utilized to address

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social problems related to both the entities present and the analytical procedures employed to detect such entities. The social dimension of analysis is often present in economy and trade, food quality, agriculture, environmental protection, fuels, defense, health (for example, quality control of medical supplies, biomedicine, health care, forensic chemistry), archaeology, space science, industrial processes and ethics (Karayannis and Efstathiou, 2012; Zolotov, 2020). Apart from chemists, other scientists, including physicists, geologists, health scientists, environmental scientists, and chemists, consider chemical analysis to be an important tool (Skoog *et al.*, 2007).

The concept of chemical analysis meets the prerequisites that are required for the construction of a conceptual profile model associated with it (Mavridi *et al.*, 2025). Recently, a preliminary classification of various ways of thinking about chemical analysis based on historical and epistemological sources (sociocultural domain) and students' alternative conceptions (ontogenetic domain) has been proposed (Table 1). These ways of thinking include the conceptualization of both material entities (the targets and/or the endpoints of analysis) and analytical procedures (Mavridi *et al.*, 2025).

The six expanded categories of ways of thinking shown in Table 1 could be considered as a “quasi” conceptual profile model of chemical analysis since primary data from students were not taken into account. Therefore, the purpose of the current work is the determination of the distinct ways of thinking about chemical analysis (zones) that constitute a conceptual profile model through the dialogic interaction of the recently proposed expanded categories of ways of thinking (Mavridi *et al.*, 2025) with primary data which comprise the microgenetic domain.

Particularly, the research questions that guided data collection, analysis and interpretation were as follows:

(1) *How does the incorporation of the microgenetic domain shape the ontological, epistemological and axiological commitments of the expanded categories of ways of thinking about*

*chemical analysis (in terms of the entities and/or analytical procedures) proposed by the sociocultural and ontogenetic domains?*

(2) *How do the expanded categories of ways of thinking about chemical analysis proposed by the sociocultural and ontogenetic domain evolve to the zones of a conceptual profile model of chemical analysis through the incorporation of microgenetic domain data?*

## Theoretical framework

According to Mortimer *et al.* (2014b), the conceptual profile framework is a methodological approach that provides insight into the diversity of students' thinking in educational settings. Different ways of thinking about a concept are represented by the zones that comprise a conceptual profile model (Mortimer *et al.*, 2014a).

The conceptual profile framework is based on the underlying premise that people think in various ways and use different modes of thinking when dealing with different situations (Mortimer *et al.*, 2014a). This heterogeneity in thinking for a certain notion exists both in the population and within individuals (Mortimer *et al.*, 2014a; da Silva Costa and dos Santos, 2022). Even though different people may think and speak in similar ways as a result of common experiences within comparable social and cultural contexts (Mortimer *et al.*, 2012), people have distinct conceptual profiles for different concepts as each zone is given a different weight; in other words, individuals' backgrounds influence their ability to employ different ways of thinking (Mortimer *et al.*, 2012) and making sense of the concept in various contexts as well (Orduña Picón *et al.*, 2020). Additionally, science itself can present multiple viewpoints on the same phenomenon since it is not a homogeneous body of knowledge. Thus, a person can have different coexisting meanings for a concept which, in appropriate contexts, can be expressed verbally (Mortimer *et al.*,

**Table 1** Expanded categories of ways of thinking about chemical analysis based on the concurrent examination of the sociocultural and ontogenetic domains

| Expanded categories of ways of thinking | Description  |
|---|--|
| Everyday analysis                       | Thinking about chemical analysis involves useful stuff or objects that are analyzed independently of theory and using the human senses, based on their explicit or object-related properties.  |
| Alchemical analysis                     | Thinking about chemical analysis is influenced by the origins of alchemy and involves materials with an essence that are analyzed using senses or simple isolation and separation procedures, while theory is manipulated or partially used.   |
| Empirical analysis                      | Thinking about chemical analysis involves elements and compounds as components that are operationally classified and determined by simple theory-based experiments in compliance with scientific method.   |
| Classical analysis                      | Thinking about chemical analysis involves elements and compounds that are determined by qualitative or quantitative experiments based on their specific chemical composition, physical or chemical properties and structure–property relationships in accordance with theoretical standards.   |
| Classical instrumental analysis         | Thinking about chemical analysis involves dynamically interacting entities having emergent physicochemical properties that are determined by accurate, sensitive, non-destructive, fast, expensive and complicated procedures based on the transformation of analytical signals and deductive explanations or predictions within (analytical) chemistry's framework. |
| Contemporary tool for society           | Thinking about chemical analysis involves entities related to social problems and determined by instrumental methods based on large data, integration of microcomputers, chemometrics, collaboration between scientific fields, compromises and empiricism as well as favorable, impartial or unfavorable opinions about it.   |



2014b). For example, one might use the word “warm” to describe a warm garment when they want to buy one rather than describing it as a good thermal insulator, which would be the case in physics class (Mortimer *et al.*, 2014b). Furthermore, scientific terms may occasionally be used in common language in ways that are not consistent with their scientific connotations. This implies that a person’s conceptual profile may contain one or more ways of thinking that are not consistent with the scientific ones (Mortimer *et al.*, 2012).

For developing a conceptual profile model, specific ways of thinking (zones) about the concept are determined (Mortimer *et al.*, 2014a) and ontological, epistemological and axiological commitments about the meaning of each different way of thinking define, establish and stabilize the zones (Mortimer *et al.*, 2014b).

Vygotsky’s model of mind requires a clear sociocultural basis (Weisner, 1987). This means that social interactions are crucial for the high mental function of conceptual thinking and the different ways of thinking about a concept are dependent on the specific sociocultural context studied (Mortimer *et al.*, 2014b; Orduña Picón *et al.*, 2020). According to Wertsch’s interpretation on Vygotsky’s work, in order to fully explain psychological phenomena, one should analyze different types of development, which Wertsch called genetic domains (Wertsch, 1985). Three of Vygotsky’s proposed genetic domains, namely the sociocultural (historical and epistemological development of a concept), ontogenetic (development of a concept in everyday life in different people) and microgenetic domains (development of a concept in microprocess of interaction in specific settings and situations), should be taken into account while developing a conceptual profile model, so as to include the variety of meanings attributed to the concept in question in all contexts and situations where it has a meaning (Wertsch, 1985; Mortimer *et al.*, 2014b).

With the above-mentioned in mind and in accordance with the theoretical and methodological bases of conceptual profile research program as suggested by its pioneers, data collection involves using many sources, rather dialogically and not chronologically, meaning that all data categories are interacting with one another at the same time (Mortimer *et al.*, 2012, 2014a). For the sociocultural genetic domain, one can study secondary literature pertaining to history of science and epistemological research on the concept, thus providing a comprehension of the challenges and shifts in the way of thinking about a particular concept and the impact of these shifts. The ontogenetic domain, on the other hand, is well-represented in studies on students’ alternative conceptions and empirical data from educational settings, both of which provide insight into how concepts are learned and developed in daily life. Last but not least, the microgenetic domain, namely the microprocesses that take place during small-scale interactions in a range of settings and situations where the concept makes sense, like a classroom, is studied using authentic data gathered through questionnaires, interviews and video recordings (Mortimer *et al.*, 2012, 2014b; da Silva Costa and dos Santos, 2022).

## Methodology

This research adopted a qualitative approach based on the conceptual profile theoretical framework. Its founders (Mortimer *et al.*, 2014a) suggest that there are two primary methodological approaches for creating a conceptual profile model. One approach is to begin with the examination of philosophical, historical and alternative conceptions sources (sociocultural and ontogenetic domains), which results in the proposal of an initial categorization of ways of thinking. These expanded categories may then assist in the analysis of students’ responses (microgenetic domain), resulting in a further refinement of the categories to establish the zones which comprise a conceptual profile model of the concept under study. However, empirical evidence might be more detailed than what sociocultural and ontogenetic domain articulates. An additional concern is the possibility of bias in the interpretation of the raw data. A different option is to start by analyzing primary data (microgenetic domain) partly inductively. Nonetheless, the obvious disadvantage of this approach is that it will result in a very poor categorization of empirical data, making it difficult to interact with historical, philosophical and sources of alternative ideas (sociocultural and ontogenetic domains). In each of these instances, we aim to mitigate the impacts of the risks we pointed out by constantly bringing together data from all three genetic domains (Mortimer *et al.*, 2014a).

In our work, we employed the first of the above-mentioned types of strategy: recent work (Mavridi *et al.*, 2025) describes the contribution of the sociocultural and ontogenetic domains in the development of a proposed conceptual profile model of chemical analysis and provides more information about data collection and analysis regarding historical, epistemological and alternative conceptions sources. In particular, the diverse ideas and views of chemical analysis identified through the study of the sociocultural and ontogenetic domains were categorized into extended categories that reflect the various ways of thinking about the concept based on how chemical analysis is perceived.

### Data collection

The microgenetic domain was explored by collecting primary data from students’ responses to questions of a semi-structured interview protocol. The interview questions are provided as SI.

The research took place in Athens, Greece. In particular, the participants of this qualitative research were 12 high school students [S] (11th grade, 16–17 years old) and 9 chemistry undergraduate students [U] (3rd year-6th semester, 20–22 years old). More specifically, high school students in Greece have already started studies on chemical content since 8th grade. Chemical analysis is mentioned across different topics (*e.g.* solutions, acids-bases, detection reactions of organic compounds) yet laboratories of public secondary schools are not very often used by students and the textbooks in use only include a small number of experimental work activities. Thus, we chose 11th grade students because by the second semester they may have a fundamental understanding of chemical



analysis for both elements and organic and inorganic compounds. Also, 3rd-year (6th semester) undergraduate chemistry students were chosen because, according to the existing curriculum, they should have successfully completed all compulsory courses offered by the field of analytical chemistry which include laboratory activities, so they will most likely possess all necessary knowledge about the entities and procedures related to chemical analysis.

We aimed to include as many different ways of thinking as possible. With that in mind and because both the high school and the university are public and no social, economic or other criteria (*e.g.* strong academic performance) were used to select participants for the study, we contend that the students are sufficiently diverse to detect a heterogeneity in speaking and thus thinking (Orduña Picón *et al.*, 2020) about the concept of chemical analysis. Additionally, because the degree of polysemy of a particular concept varies between educational levels and since most of the ontogenetic domain's sources dealing with alternative conceptions involved both secondary school and university students, both educational levels are represented among the students (El-Hani *et al.*, 2015).

We employed a semi-structured interview based on chemical analysis tasks as our research instrument. We anticipated that these tasks would encourage students to reveal their ontological, epistemological and axiological commitments of the zones in their conceptual profiles, potentially accompanied by any concerns about them (Coutinho *et al.*, 2014). After all, when compared to data collected *via* other means such as questionnaires, interview data provide a deeper understanding of the ways students think (Mortimer *et al.*, 2014a).

A pilot study was conducted in which the interview protocol was tested twice with 11th grade students to identify any understanding issues that may develop in the lower level of education. All necessary modifications were made in order to ensure effective implementation of the instrument to both high school and university students. The phrasing and content of the questions asked was thoroughly considered to make sure that the answers were not biased.

The interview protocol consists of three general questions about chemical analysis followed by more specific questions (Baltieri *et al.*, 2021). The specific questions concern a certain task addressing the problem of the identification of five unknown materials, namely anesthetic, white wine, white vinegar, perfume and plastic film. In addition to being familiar to students from their daily lives, these materials contain simple organic compounds (not necessarily as the main component), namely ethane, ethanol, ethanoic acid, 1-propanol and polyvinyl chloride (PVC), respectively. Except for PVC, which however is one of the simplest polymers and is taught in schools, these compounds contain two or three carbon atoms and the pilot study revealed that students handled all of them without any problems. In order to avoid an overpowering effect of appearance (*e.g.* color) on the response, the vinegar and wine are chosen to be white rather than red or rosé.

Initially, participants carried out this task without any help, so we received insight into their overall approach to analysis

without any kind of stimulus. To prevent responses from being constrained by a lack of students' pertinent knowledge, particularly regarding the lower educational level, students were then given access to information about the materials and compounds, including their organoleptic characteristics, function, origin, physical characteristics, molecular and structural formula, some chemical properties (reactions),  $^{13}\text{C}$ -NMR and specifics of their applications in society. Since secondary school students had little prior knowledge regarding spectra, we gave them a brief explanation of the approach's operating principles and addressed any comprehension difficulties. All types of information were delivered to students concurrently rather than sequentially, ensuring that participants always had access to all information and could use any kind of information in any question. Thus, construct validity was not compromised. Following that, they were given the same task once more, this time with guiding questions that highlighted the conceptual profile's dimensions. In general, we asked them about the nature of these entities and analytical procedures (the ontological dimension), how knowledge about them is constructed (the epistemological dimension) and what assessments and judgements about them are made (the axiological dimension) (Sodre and Mattos, 2022). Lastly, as a result of the pilot study, a broad question concerning chemical analysis was employed. The interview protocol is available in SI.

We acknowledge that our specific methodological approach including the design of the interview protocol may have an impact on our findings. To mitigate this risk, we closely adhered to the guidelines of the founders of the conceptual profile theoretical framework and the methodological research program associated with it (Mortimer *et al.*, 2012, 2014a, 2014b) as well as the research tools employed in previous works in the microgenetic domain (Coutinho *et al.*, 2014; Sepulveda *et al.*, 2014; do Amaral *et al.*, 2018; Sodre and Mattos, 2022). After all, constructing a conceptual profile model involves determining the ontological, epistemological and axiological commitments of each zone in order to identify as many distinct ways of thinking about a given concept as possible. Therefore, the variety of tasks and questions should be viewed as encouraging the expression of all diverse ways of thinking rather than restricting or biasing it. Because several meanings of a concept may coexist in a person and be utilized in particular contexts where they make sense (Mortimer *et al.*, 2014b), the variety of tasks and information that students experience seeks to encourage them to think about a concept in different ways, without being limited by any lack of relevant knowledge.

The interviews took place during April and May 2025. The researcher who conducted them was unknown to the students. The interviews were made in a room in which only the interviewer and the interviewee were present. Students participated voluntarily in the study and, for ethical precaution, the guardians' consent was acquired for participants who were under the age of 18. The researcher ensured the confidentiality of the data as well as the identities of those being interviewed. It was also stated that the research aimed at the identification of their thinking and not to assess whether their answers were correct



or incorrect. The average interview duration was ca 25 min with the longest lasting approximately 35 minutes. All interviews were recorded (obviously with the consent of the participants or their legal guardians) and subsequently transcribed for analysis. All data in this work were gathered after obtaining official approval for the conduct of this research by the ethics committee of the higher education institution with which the corresponding author is affiliated.

### Data analysis

An inductive–deductive qualitative data analysis approach was adopted (Mortimer *et al.*, 2012). In particular, the expanded categories of ways of thinking about chemical analysis already identified through the study of sociocultural and ontogenetic domains (Mavridi *et al.*, 2025) were used as a coding framework for the dialogic analysis of primary data collected from student's interviews (microgenetic domain) (Fig. 1) (Mortimer *et al.*, 2014a). These initial categories served as a foundation for classifying the different answers to the questions, but we were also flexible to the propositions of new categories that emerged from the responses themselves and to the possibility that categories that were absent from the students' answers might eventually not be regarded as zones, as shown in the Results section (Coutinho *et al.*, 2014). Additionally, we considered the chance that some of these answers might fall within more than one zone (Aguiar *et al.*, 2018; do Amaral *et al.*, 2018).

Every piece of data was examined multiple times so as to enhance the reliability of analysis (Solsona *et al.*, 2003). To ensure the validity of the analysis, all authors analyzed independently four randomly selected transcripts from university students and then they met to discuss coding and resolve any disagreements. Following the conversation, the first two authors independently conducted analysis of all data obtained from university students. Once more, disagreements were

discussed until agreement was obtained. The process for analysis of secondary students' data was the same (Pereira and Mortimer, 2025).

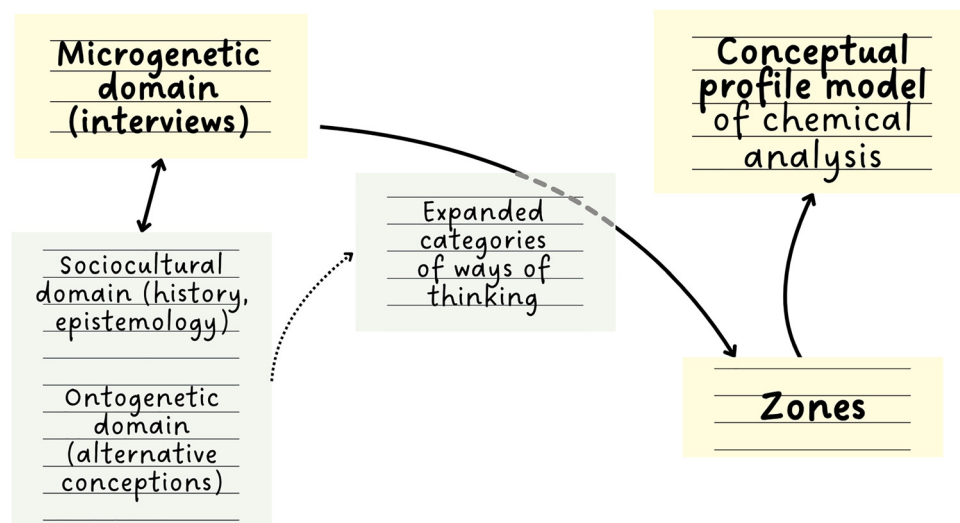
## Results and discussion

This section outlines the findings of the current study, which are the zones of a conceptual profile model of chemical analysis. These zones are established as an evolution of the already proposed expanded categories of ways of thinking about chemical analysis, depicted in Table 1 (Mavridi *et al.*, 2025). The expanded categories of ways of thinking about chemical analysis with their commitments had been emerged by a dialogue between sociocultural and ontogenetic domains, while zones of the proposed conceptual profile model of chemical analysis by a dialogue between sociocultural, ontogenetic and microgenetic domains.

To help readers understand how commitments have been refined through interaction with microgenetic domain data, each commitment's refinement along with the evolution of expanded categories into zones is displayed in a table format. Excerpts from the interview are presented to support this process due to dialogue between previous findings with microgenetic domain data. Examples in which the answer appears without the associated question are those in which either the question is easily deduced from the answer or the excerpt is only a part of a participant's thinking that is not closely related to what is being asked at the time.

### Zone: everyday analysis

**Ontological commitments.** Following the dialogic interaction of the findings from the analysis of sociocultural and ontogenetic domains data with those of microgenetic domain,



**Fig. 1** The refinement of commitments through the dialogical interaction of microgenetic data with sociocultural and ontogenetic data leads to the establishment of the zones of a proposed conceptual profile model of chemical analysis. Grey background indicates steps that have already been conducted (Mavridi *et al.*, 2025).



**Table 2** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of everyday analysis zone

| Everyday analysis               | Expanded category   | Zone                              |  |  |
|---------------------------------|---|-----------------------------------|--|--|
|                                 |   | Dialogue with microgenetic domain |  |  |
|                                 | Dialogue between sociocultural – ontogenetic domains  | YES                               | NO   | NEW  |
| Entities                        | Matter as categories or types of stuff and objects  | • Stuff, objects                  | • Categories or types                                  | • Materials instead of matter                  |
| Procedures                      | Separation of matter into basic parts, simple, mostly employing human senses  | • Simple<br>• Human senses        | • No distinction between separation and identification | • Not always in labs (ontological commitments) |
| Refined ontological commitments | Materials as stuff or objects analyzed with simple procedures employing human senses, not necessarily in laboratories |                                   |  |  |

the ontological commitments of “everyday analysis” were refined (Table 2).

More precisely, we substitute the term “matter” for “materials” in the ontological commitment of “everyday analysis” zone, since students, as most chemists do, frequently discuss the concrete materials that chemistry deals with rather than the more abstract and philosophical notion of matter (Wasserman, 2021), as seen in the following example:

[Part 1, without detailed information on the tables]  
Interviewer: *How can we find out which material is in each container?*

U1: *We could smell the wine, vinegar and perfume and we distinguish them, the anesthetic, um... the plastic film, I guess, looks different from the others... the anesthetic, I guess, will be the one that's left over, so that's how I would tell them apart.*

They indeed think of materials as nothing more than stuff or objects; however, they rarely notice categories or types of them.

[Part 2, after reading the tables] U7: *... We used to think that wood, for example, was an element of nature...*

[Part 2] Interviewer: *What do you think makes a material what it is?*

S7: *... Once you know what a material is, you understand its use. For example, you can't just go ahead and chop stuff with a banana...*

[Part 1] Interviewer: *What comes to mind when you hear the word “analysis”?*

S10: *... Chemical analysis is to cut something open and look inside...*

Also, we now prefer to use the expression “materials... analyzed” rather than “matter... which can be separated” because students do not make distinction between separation and identification, thus making the term “analysis” more appropriate.

[Part 1] U2: *... I think we would recognize the perfume by its scent...*

[Part 1] U3: *... vinegar, perfume and wine are all easily distinguished by smell...*

Many students' responses confirm that these simple analytical procedures rely heavily on the use of human senses:

[Part 1] Interviewer: *How can we find out which material is in each container?*

S2: *... by touching, by smelling and, if we know they are edible, we can taste them...*

S4: *... If the container is transparent, it will be visible to the naked eye...*

Additionally, for this way of thinking the place where analysis is conducted is not necessarily a laboratory, as already has been indicated by sociocultural and ontogenetic domains:

[Part 1] Interviewer: *How can we find out which material is in each container?*

S7: *For example, for wine, I think I would go for its taste... you can use these properties in your daily life...*

This constitutes rather an ontological than an epistemological commitment (which had been considered as such in the previous stage of constructing the conceptual profile model of chemical analysis) because the setting is more reflective of how analysis is perceived (in terms of both entities investigated and procedures employed) than of the process of knowledge construction.

**Epistemological commitments.** Dialogue between data from all three genetic domains (Table 3) agrees that when thinking about chemical analysis, most students employ the use of senses to observe explicit or object-related properties.

The following examples are indicative:

[Part 2] Interviewer: *Describe a way you would suggest finding out which material is placed in each container.*

U4: *... At first, I observe them again and the film seems different from the anesthetic...*

S5: *... I'd take the container next; I would shake it to determine whether it was liquid, gas or solid...*

[Part 2] Interviewer: *If we could see inside a material, what would we see?*

S10: *Small pieces that together create this texture.*

Furthermore, they typically use the purpose and function or even the origin of materials to gain a better understanding of them:

[Part 2] Interviewer: *What do you think makes a material what it is?*

S7: *Its properties... When you use it, something will happen. I know that the anesthetic will... you will fall asleep, the wine will make you drunk, the vinegar will make you feel a little bitter... the cologne... Use makes a material what it is.*



**Table 3** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of everyday analysis zone

|  | Expanded category  | Zone   |   |   |
|--|--|--|---|---|
|  |  | Dialogue with microgenetic domain  |   |   |
| Everyday analysis                                    | Dialogue between sociocultural – ontogenetic domains   | YES  | NO  | NEW   |
| Knowledge construction about entities and procedures | Independently of theoretical ideas, use of senses – direct observation of explicit or object-related properties, not necessarily in a laboratory | <ul style="list-style-type: none"> <li>• Use of senses</li> <li>• Explicit or object-related properties</li> <li>• No use of theory</li> </ul> | <ul style="list-style-type: none"> <li>• Lab (ontological commitments)</li> </ul> | <ul style="list-style-type: none"> <li>• Functions, origin</li> </ul> |
| Refined epistemological commitments                  | Use of senses – observation of explicit or object-related properties, functions and origin, independently of theory                              |  |   |   |

[Part 2] Interviewer: *How did you think in order to find out which material exists in each container?*

U6: *...It [origin] could help me because if someone tells me, "You know, we got this from such-and-such a sample of natural gas and oil", I immediately understand what I might have...*

U9: *...I might recognize it from its behavior...*

Responses support the already suggested epistemological commitment that theory has no bearing on the process of knowledge creation since no theoretical concepts about the entities that comprise the endpoints of analysis are discussed. The passage that follows illustrates how students' knowledge of chemistry has no impact on their understanding:

[Part 2] Interviewer: *How did you think in order to answer the question regarding what a material is made of?*

S8: *Since I'm not very good at chemistry, I thought of examples from everyday life that are simpler and, I believe, easier for everyone to understand.*

**Axiological commitments.** Table 4 shows the outcome of the dialogic interaction between the microgenetic-sociocultural-ontogenetic domains in terms of the zone's axiological commitments.

In accordance with sociocultural and ontogenetic domains, students believe that analyzing materials that are useless for their everyday life is pointless.

[Part 1] Interviewer: *What materials can be analyzed by employing chemical analysis?*

S4: *We can analyze materials that interest us and are actually useful to us.*

We choose to exclude the term "professional needs" from this commitment because most participants do not express it, which is understandable given that they do not have a day job. In addition to being helpful, the materials being analyzed are also considered simple, as students seem to think that only these materials can be analyzed by observation and the use of senses.

[Part 2] U5: *...Ethanol and vinegar are clear in color and, well, ethanol and vinegar are obvious, so the fragrance is all I need to tell them different...*

Useful exemplary materials are often mentioned, as we already read in a previous response:

[Part 2] U7: *...We used to think that wood, for example, was an element of nature...*

Procedures are thought to be fast, easy, straightforward to implement and simple to comprehend:

[Part 2] Interviewer: *Why is the procedure you proposed important?*

S5: *...I feel that it is a simple and quick approach...*

[Part 2] Interviewer: *Why did you use this piece of information?*

S1: *...It's easier... it seems easier for me to think about these qualities. And that came to me straight away, I mean, let's talk about the taste... I consider it quite characteristic... and the same goes for the smell of vinegar...*

**Table 4** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of everyday analysis zone

|                                 | Expanded category   | Zone   |  |  |
|---------------------------------|---|--|--|--|
|                                 |   | Dialogue with microgenetic domain  |  |  |
| Everyday analysis               | Dialogue between sociocultural – ontogenetic domains  | YES  | NO   | NEW  |
| Evaluations and judgements      | Useful materials and procedures for daily and professional needs  | <ul style="list-style-type: none"> <li>• Useful materials</li> <li>• Useful procedures</li> <li>• Daily lives</li> </ul> | <ul style="list-style-type: none"> <li>• Professional needs</li> </ul> | <ul style="list-style-type: none"> <li>• Simple materials</li> <li>• Simple, fast, easy, straightforward procedures</li> <li>• Subjective, inaccurate, dangerous procedures</li> </ul> |
| Refined axiological commitments | Only simple and useful materials are analyzed with fast, easy, simple, yet subjective, inaccurate, dangerous procedures |  |  |  |



Yet there are several concerns about their objectivity, accuracy and potential dangers:

[Part 2] S2: ...*materials' properties aren't something I would use because we might not be able to differentiate between yellow, pale yellow etc...*

[Part 2] U5: ...*because it's also subjective; for example, let's say they have a different smell but what if I think they smell the same?*  
...

[Part 2] U5: ...*Unlike here, any method, not necessarily involving a machine, is more reliable and gives me a very high degree of accuracy...*

[Part 2] U3: ...*The disadvantage is that it is not advised to taste or smell the materials we have...*

### Zone: alchemical analysis

**Ontological commitments.** Based on the dialogic interaction between data from all three genetic domains (Table 5), we claim that when someone thinks about chemical analysis as alchemical, they perceive that materials have an inherent essence.

This is quite apparent in the following dialogue:

[Part 2] Interviewer: *When materials undergo a chemical reaction, what changes and what stays the same?*

S10: *Well, there will always be something, a component, or even tiny parts that will never change. Also, the molecules? I'm not sure...*

Interviewer: *What do you mean?*

S10: *Nothing is completely changed; there is still a remnant of the previous state.*

This inherent essence is lost when the material is transformed into something invisible or “non-material”, like gases.

[Part 2] S7: ...*It [ethane] is a gas, so there is nothing...*

Microgenetic domain data also supports the fact that the analytical procedures that students consider present when thinking about chemical analysis as alchemical are based on their senses or through observation of simple experiments.

[Part 2] S7, U8: ...*If we could see inside a material, we would probably see the color of the molecules...*

[Part 2] Interviewer: *What changes in materials when a chemical reaction occurs and what remains the same?*

U1: *Everything can either change or remain the same.*

Although the description of the essence as “principles”, “elements”, “substances” and “contraries” was accurate for the

alchemists of that period (Leicester, 1971; Pérez-Bustamante, 1997), we did not find analogous descriptions in participants' responses. Thus, we decided to omit these descriptive phrases from the ontological commitments. For the same reason, we avoid using the word “specific” as descriptive of analytic processes.

**Epistemological commitments.** As shown in Table 6, the microgenetic domain also suggests that knowledge construction about the “essence” of entities is based on the observation of essential and additive properties of materials; however, it is unclear whether it takes place only through the use of human senses.

The following students' responses are indicative:

[Part 2] Interviewer: *What do you think makes a material what it is?*

S10: *The presence or absence of different elements is crucial because a larger concentration of gases results in a different composition.*

U7: ...*some special properties that some substances possess; for example, I am aware that vinegar has a particular scent...*

In accordance with sociocultural and ontogenetic domains, students either do not employ relevant theoretical concepts at all or only partially use them. This is demonstrated by the following arbitrary responses provided by students, which are not grounded in theory learned during chemistry courses, although students referred to some theoretical ideas like “functional group”.

[Part 2] Interviewer: *If we could see inside a material, what would we see? What is it made of?*

S5: ...*I believe that these compounds consist of microorganisms that are man-made, designed for a specific use; let's say ethane is different from ethanol, for different uses...*

[Part 2] Interviewer: *How did you think in order to find out which material exists in each container?*

U7: ...*there will be a functional group on the specific compound, which alone can give the correct result and will not be found in any other compound...*

The responses contained no indication of theoretical modification and, since this phrasing conveys intent and has a negative tone, we decided not to include it in the commitments. The same applies to the lack of awareness of findings and the primitive categorization of entities, which were previously suggested by sociocultural and ontogenetic domains.

**Table 5** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of alchemical analysis zone

|                                 | Expanded category   | Zone                                 |  |                                      |
|---------------------------------|---|--------------------------------------|--|--------------------------------------|
|                                 |   | Dialogue with microgenetic domain    |  |                                      |
|                                 |   | YES                                  | NO   | NEW                                  |
| Alchemical analysis             | Dialogue between sociocultural – ontogenetic domains  |                                      |  |                                      |
| Entities                        | Materials which have essence (“principles”, “elements”, “substances”, “contraries”)               | • Materials have an inherent essence | • Principles, elements, substances, contraries |                                      |
| Procedures                      | Specific, simple  | • Simple                             | • Specific                                     | • Human senses or simple experiments |
| Refined ontological commitments | Materials having an essence analyzed with procedures employing human senses or simple experiments |                                      |  |                                      |



**Table 6** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of alchemical analysis zone

|  | Expanded category  | Zone  |   |   |
|--|--|---|---|---|
|  |  | Dialogue with microgenetic domain   |   |   |
| Alchemical analysis                                  | Dialogue between sociocultural – ontogenetic domains   | YES   | NO  | NEW   |
| Knowledge construction about entities and procedures | Modifying, partially using or independently of theory, use of senses – direct observation of essential/additive properties, primitive categorization, lacking awareness of some findings, constant repeating | <ul style="list-style-type: none"> <li>• Based on essential and additive properties</li> <li>• Partial use or no use of theory</li> </ul> | <ul style="list-style-type: none"> <li>• Constant repeating</li> <li>• Theory modification</li> <li>• Primitive categorization</li> <li>• No awareness of findings</li> </ul> | <ul style="list-style-type: none"> <li>• Not just human senses</li> </ul> |
| Refined epistemological commitments                  | Observation of essential and additive properties, partially using or independently of relevant theory  |   |   |   |

**Table 7** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of alchemical analysis zone

|                                 | Expanded category   | Zone   |   |     |
|---------------------------------|---|--|---|-----|
|                                 |   | Dialogue with microgenetic domain  |   |     |
| Alchemical analysis             | Dialogue between sociocultural – ontogenetic domains  | YES  | NO  | NEW |
| Evaluations and judgements      | Influenced by the origins of alchemy, fusing domains of experience-knowledge, positive–negative attitudes | <ul style="list-style-type: none"> <li>• Confusion between experience and knowledge</li> </ul> | <ul style="list-style-type: none"> <li>• Influence of alchemy's origins</li> <li>• Positive–negative attitudes</li> </ul> |     |
| Refined axiological commitments | Fusing domains of experience-knowledge  |  |   |     |

**Axiological commitments.** In the microgenetic domain, it must be emphasized how experience and knowledge are frequently muddled in students' thinking, as previously noted in the sociocultural and ontogenetic domains (Table 7).

[Part 2] Interviewer: *What remains the same in materials when a chemical reaction occurs?*

S1: *...Some elements may outweigh other elements and neutralize them...*

Furthermore, although the sociocultural domain strongly suggested evaluations and beliefs influenced by the history of alchemy, particularly its philosophical, mystical, spiritual and supernatural background, which are derived from Greek philosophy, Egyptian technology and Eastern mysticism (Leicester, 1971), we were unable to locate those thoughts in students' responses, so we did not include them in the axiological commitments. The same applies to positive and negative attitudes towards chemistry which were detected in the sociocultural and ontogenetic data but not in students' responses related to alchemical analysis.

### Zone: empirical analysis

**Ontological commitments.** Given the indications of the ontological commitments from the sociocultural and ontogenetic domains and their interaction with microgenetic domain data

(Table 8), students consider elements and compounds to be constituents of both pure materials and mixtures.

This can be seen from the following excerpts.

[Part 1] Interviewer: *What other words spontaneously come to mind when you hear the word "analysis"?*

S2: *Analysis of compounds or elements.*

[Part 1] Interviewer: *What materials can be analyzed by employing chemical analysis?*

S3: *...[we can analyze] carbon, carbon compounds, water...*

[Part 1] Interviewer: *What are your thoughts and what comes to mind when you hear the words "chemical analysis"?*

U3: *It is the qualitative and quantitative composition of a sample. In short, what it contains, what compounds are there and in what quantity.*

U7: *I would describe it [analysis] as determining the content of a solution, what distinct compound exists in a material or solution...*

[Part 1] Interviewer: *What materials can be analyzed by employing chemical analysis?*

S8: *...We can use chemical analysis to analyze a mixture, such as its composition, chemical substances, and so on...*

Additionally, students would analyze these components using basic laboratory procedures, as evidenced from the following discourse:



**Table 8** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of empirical analysis zone

|                                 | Expanded category  | Zone  |  |   |
|---------------------------------|--|---|--|---|
|                                 |  | Dialogue with microgenetic domain   |  |   |
| Empirical analysis              | Dialogue between sociocultural – ontogenetic domains   | YES   | NO   | NEW   |
| Entities                        | Elements and compounds as components of materials, objects, solutions  | <ul style="list-style-type: none"> <li>• Elements, compounds</li> <li>• Components of pure materials, mixtures</li> </ul> | <ul style="list-style-type: none"> <li>• Components of objects, solutions</li> </ul> |   |
| Procedures                      | Simple, experimental   | <ul style="list-style-type: none"> <li>• Simple, experimental</li> </ul>  |  | <ul style="list-style-type: none"> <li>• Basic</li> </ul> |
| Refined ontological commitments | Elements and compounds as components of mixtures or pure materials analyzed with basic experimental procedures |   |  |   |

[Part 2] Interviewer: *Describe a method you would use to find out which material is placed in each container.*

S7: *First, I would boil them to observe at what temperatures they change form... or I would add something to them, such as sodium, and see whether they react...*

Interviewer: *How do you see that?*

S7: *It will either bubble or nothing will happen... I can test its acidity... there are specific strips that you may put in and remove... and they change color...*

As previously noted (microgenetic domain of the zone referring to “Everyday analysis”), it is the ontological rather than the epistemological commitment which refers to the location of analysis (*i.e.* the laboratory).

[Part 1] Interviewer: *What materials can be analyzed by employing chemical analysis?*

S4: *In general, chemical components that can be found in nature.*

Interviewer: *How do we analyze a material?*

S4: *Through experiments.*

Interviewer: *What kind of experiments?*

S4: *I think they can only be performed in laboratories.*

**Epistemological commitments.** With respect to the epistemological commitments of this zone, Table 9 displays the

results of the dialogic interaction between the microgenetic, sociocultural and ontogenetic domains.

Specifically, thinking about laboratory procedures depends on the observation and detection of the physical and chemical properties of mixtures and pure materials.

[Part 1] U6: *...I can also do it with observation. That is, I can observe color changes, indicators, anything...*

[Part 2] Interviewer: *How did you think in order to answer the question regarding what it is made of?*

U1: *There are specific tests... we see their properties and, because they have been known for a long time and we have tables of known properties, we can compare melting points, boiling points, textures, densities, solubilities...*

As shown in the following extract, the interaction between components results in materials with new and distinct properties which are not present or predictable from the properties of the individual components themselves. These properties are called emergent and they only apply to mixtures or pure materials and not to their constituent parts (Luisi, 2002). This is in line with the already proposed commitment of the expanded category of empirical analysis based on the dialogue between sociocultural and ontogenetic domains.

[Part 2] Interviewer: *What do you think causes these properties?*

**Table 9** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of empirical analysis zone

|  | Expanded category  | Zone  |   |  |
|--|--|---|---|--|
|  |  | Dialogue with microgenetic domain   |   |  |
| Empirical analysis                                   | Dialogue between sociocultural – ontogenetic domains   | YES   | NO  | NEW  |
| Knowledge construction about entities and procedures | Theories, simple experiments carried out in laboratories – scientific method, determination of emergent properties, operational categorization | <ul style="list-style-type: none"> <li>• Emergent properties</li> <li>• Operational classification</li> <li>• Theory</li> </ul> | <ul style="list-style-type: none"> <li>• Determination</li> <li>• Lab (ontological commitments)</li> <li>• Scientific method (axiological commitments)</li> </ul> | <ul style="list-style-type: none"> <li>• Observation, detection</li> <li>• Physical, chemical properties</li> <li>• Vaguely based on theory</li> </ul> |
| Refined epistemological commitments                  | Observation and detection of emergent physical and chemical properties, operational categorization, vaguely based on theory                    |   |   |  |



S10: ...because it [the material] is made up of various other components and the combination of these results in something new, a different property...

These emergent properties do not distinguish compounds from mixtures. Given that the notion of determination is mainly referred to the structure of a substance (Talanquer, 2016), the terms “observation” and “detection” based on the predominance of the empirical nature of analysis are more relevant than the term “determination”. Additionally, mixtures and materials are operationally classified – that is, according to their properties rather than their structure. The following passage is an example of incorporating the operational categorization of acids/bases in one’s thinking:

[Part 2] U3: *The knowledge of the properties of materials may assist me with a problem that I may have. That is, I may be dealing with a problem and need an acid or a base...*

Also, knowledge and thinking about both entities (materials, mixtures, elements and compounds) as well as procedures are vaguely theory-based, since previous findings are sometimes cited rather than specific theoretical explanations.

[Part 2] Interviewer: *Why did you use this piece of information?*

U1: *We observe the properties and because these have been established for a long time and we have some tables with known properties, we can compare them.*

Evidence of the scientific method was mostly found in judgments and evaluations, so it is only referenced in the axiological commitments.

**Axiological commitments.** Table 10 shows the outcome of the dialogic interaction between the microgenetic-socio-cultural-ontogenetic domains in terms of the zone’s axiological commitments.

Students’ responses reveal that, as already suggested, evaluations about chemical analysis are usually focused on how well the knowledge of entities agrees with theory and how closely the (more or less) experimental techniques adhere to the scientific method.

[Part 2] Interviewer: *How did you think in order to answer the question regarding what the material is made of?*

S2: *Based on their reactions and results; observing the findings and drawing conclusions...*

[Part 1] Interviewer: *What comes to mind when you hear the words “chemical analysis”?*

S1: *...Let us say experiments come to mind. That through specific experiments, you try to find and explain certain data, facts and...*

Furthermore, some respondents’ express concerns about the ease of use

[Part 2] S9: *...It is easier to do it using your eyes, because you can see it...*

[Part 2] U2: *...The drawback of reactions is that they require equipment such as tubes and reagents...*

as well as the objectivity and accuracy of methods.

[Part 2] S2: *...Reactions give you more certainty about something. With density, I suppose you are totally sure of something; I believe you can be safe when measuring a substance’s density. The boiling point also produces certain outcomes...*

[Part 2] U3: *If we used the boiling point... we wouldn’t be 100% certain, so we’d utilize it as a first step, as an initial separation...*

### Zone: compositional analysis

**Ontological commitments.** Table 11 depicts the outcome of the dialogic interaction between the microgenetic-socio-cultural-ontogenetic domains in terms of the zone’s ontological commitments.

Students’ responses confirm the previous findings, namely that this way of thinking includes the perception of specific chemical composition of substances (elements and compounds), namely: atoms, molecules and functional groups.

[Part 2] S7: *...Inside a material, we get to see the bonds between molecules; in fact, we can see the atoms that make up the molecules and maybe the compounds...*

[Part 2] U2: *...They [materials] are composed of atoms. Now, in my mind, I picture them as tiny balls, but I do not believe that is how they are; I cannot imagine precisely what they might look like...*

[Part 2] S11: *...The anesthetic ethane, for instance, consists of two atoms of carbon and hydrogen. However, ... ethanol also has two carbon atoms, but it differs from ethane in that it also has an OH...*

These elements and compounds are examined using certain classical experimental procedures carried out in laboratories.

[Part 1] U7: *...using cation precipitation, for instance, to determine which cations are present in solutions, ..., volumetric measurements could be used for more quantitative purposes...*

**Table 10** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of empirical analysis zone

|                                 | Expanded category   | Zone  |    |  |
|---------------------------------|---|---|----|--|
|                                 |   | Dialogue with microgenetic domain   |    |  |
|                                 |   | YES   | NO | NEW  |
| Empirical analysis              | Dialogue between sociocultural – ontogenetic domains  |   |    |  |
| Evaluations and judgements      | Based on theory and the compliance with scientific method   | <ul style="list-style-type: none"> <li>Compliance with theory</li> <li>Compliance with scientific method</li> </ul> |    | <ul style="list-style-type: none"> <li>Concerned about ease of use, objectivity, accuracy</li> </ul> |
| Refined axiological commitments | Evaluations based on compliance with theory and scientific method, concerns about easiness, objectivity, accuracy |   |    |  |



**Table 11** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of compositional analysis zone

| Compositional analysis          | Expanded category   | Zone   |   |  |
|---------------------------------|---|--|---|--|
|                                 |   | Dialogue with microgenetic domain  |   |  |
| Entities                        | Dialogue between sociocultural and ontogenetic domains  | YES  | NO  | NEW  |
| Procedures                      | Elements and compounds with specific chemical composition (atoms, molecules) – static structures, divided into groups | <ul style="list-style-type: none"> <li>• Atoms, molecules: components of elements, compounds</li> <li>• Specific chemical composition</li> </ul> | <ul style="list-style-type: none"> <li>• Structure</li> <li>• Groups (epistemological commitments)</li> <li>• Simple</li> </ul> | <ul style="list-style-type: none"> <li>• Functional groups</li> <li>• Classical</li> </ul> |
| Refined ontological commitments | Simple experimental   | Elements and compounds with specific chemical composition (molecules, functional groups, atoms) analyzed with classical experimental procedures  |   |  |

**Table 12** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of compositional analysis zone

| Compositional analysis                               | Expanded category  | Zone  |  |   |
|--|--|---|--|---|
|  |  | Dialogue with microgenetic domain   |  |   |
| Knowledge construction about entities and procedures | Dialogue between sociocultural – ontogenetic domains   | YES   | NO   | NEW   |
| Refined epistemological commitments                  | Core chemistry concepts, fixed and mostly explicit physical and chemical properties, structure–property relationships, compositional categorization, emphasis on experimentation, accessibility of results | <ul style="list-style-type: none"> <li>• Chemical concepts</li> <li>• Fixed physical–chemical properties</li> <li>• Structure–property relationships</li> <li>• Compositional categorization</li> </ul> | <ul style="list-style-type: none"> <li>• Explicit properties</li> <li>• Emphasis on experimentation</li> <li>• Accessibility of results</li> </ul> | <ul style="list-style-type: none"> <li>• Chemical theories</li> </ul> |
|  | Determination of fixed physical and chemical properties, structure–property relationships, compositional categorization, based on chemical theories and concepts   |   |  |   |

Since the structure of these entities cannot be ascertained by classical methods alone, we do not discuss it in this zone.

**Epistemological commitments.** Our analysis of the microgenetic domain data in dialogic interaction with sociocultural and ontogenetic domain data (Table 12) revealed that chemical theories and concepts provide a solid foundation for the knowledge construction regarding entities and processes.

More precisely, the elements and compounds in question are identified based on their fixed physical and chemical properties (reactions).

[Part 2] U2: ... You need to perform tests, whether chemical or boiling point, solubility, to figure out what groups there are, because all of this is due to the functional groups...

[Part 1] U6: ... You understand, together with the characteristic reaction, ... if you have two isomers, there will undoubtedly be a characteristic reaction to help me determine which is which...

Even though the history and epistemology of chemical analysis as well as some of the students' alternative conceptions from the ontogenetic domain suggest that these properties should be explicit, this is not always the case in students'

responses and, therefore, we decided to omit this characterization from the epistemological commitments. Furthermore, structure–property relationships have a significant impact on this way of thinking, as one can assume from the following excerpts:

[Part 2] S3: *It's liquid because I believe the carbon atoms aren't as close in proximity. The bonds in gases are farther apart, whereas solids are more intimately connected.*

[Part 2] Interviewer: *What do you think to be the cause of these properties?*

S7: *Hmmm... What they are, how many carbons they contain and what makes them up.*

It is critical to note that the term “structure” refers solely to the identification of the molecular and empirical formulas of elements and compounds as well as their functional groups and not the knowledge of structural formulas or configurations. Also, we consider the categorization of elements and compounds based on their composition as an epistemological commitment instead of mentioning these groups in the ontological commitments because we judge that they are more indicative of the knowledge construction process.



[Part 2] Interviewer: *What changes in materials when a chemical reaction occurs and what remains the same?*

U2: *...If we had an aldehyde or ketone, it could turn into an acid, meaning that the atoms would be the same but not connected in the same way...*

Additionally, the emphasis on experimentation and the accessibility of results in the commitment were not noted in the participants' responses, thus it is not proposed as a commitment.

**Axiological commitments.** In terms of the zone's axiological commitments, Table 13 displays the results of the dialogic interaction between the microgenetic, sociocultural, and ontogenetic domains.

We revised the axiological commitment without significantly altering its meaning to clarify the basis of the evaluations, which is compliance with standards

[Part 1] U2: *...There is a standard which indicates that this is what it is, so if we find an exception from this, it is not, for example, ethane...as well as chemical notions and theories. This can be seen by the following passages that refer to theoretical concepts and chemical components:*

[Part 2] Interviewer: *What is the advantage of using molecular formulas?*

S9: *If you know the elements and have a fundamental understanding of high school chemistry, you can understand what each container contains using these [molecular formulas].*

[Part 2] U6: *...In fact, the key difference between chemical and physical processes is that chemical processes include the breaking and formation of new bonds. In other words, in physics, the composition remains unchanged, whereas in chemical reactions, it changes.*

Some students believe that this way of thinking enhances overall chemical thinking, and this is evident from their responses on the final question of the interview protocol: [Part 2] *"Many people argue that [...] the classical (older) methods [...] are no longer necessary and do not need to be taught in schools or universities. What are your thoughts about this? What is your opinion?"*

S3: *It is very important to have knowledge on the composition of materials because in this way, we understand more what we are doing...*

U2: *...also, it [the employment of classical methods] is a course of thinking...*

U6: *...classical methods teach you how to think...*

U7: *...The characteristic reactions prompt you to ponder a bit more...*

Students' responses specify the interconnection between synthesis and analysis, already detected in the sociocultural domain (Klein and Ragland, 2014).

[Part 2] U6: *...When we understand the building blocks, the basic building blocks, then we can make more complex compounds...*

Additionally, many participants expressed concerns about specific features of the methods, such as speed, cost and amount of work required, use of hazardous materials, accuracy and reliability; however, the sociocultural and ontogenetic domains' evaluation of procedures as complex was not detected.

[Part 2] S2: *...with the reactions [the process] becomes faster...*

[Part 2] U6: *...some reactions can be really slow...*

[Part 2] U3: *...The disadvantages are that we waste materials, which inevitably means we waste money... Also, it requires a lot of effort.... I don't know if some of them are dangerous to carry out... chemicals may have negative effects on our health when we come in contact with them.... Among the advantages, that we can see the separation more clearly? That we can see that we actually have, say, ethanol. Ah! And among the disadvantages is that something could go wrong, causing us to draw incorrect conclusions...*

[Part 2] U7: *...a random reaction, which may be violent enough, is not the most reliable method of identifying substances...*

Overall, we consider compositional analysis to be a distinct zone from empirical analysis, rather than merely a refinement of it, because their fundamental difference is the prevalence of the concept of chemical composition in compositional analysis. This is evident in all commitments of these two zones. Thus, entities in compositional analysis have a certain chemical composition, which is determined using specific procedures related to this composition (ontological commitments). These

**Table 13** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of compositional analysis zone

|                                 | Expanded category   | Zone   |  |   |
|---------------------------------|---|--|--|---|
|                                 |   | Dialogue with microgenetic domain  |  |   |
| Compositional analysis          | Dialogue between sociocultural – ontogenetic domains  | YES  | NO   | NEW   |
| Evaluations and judgements      | Based on core chemistry entities, standards-theoretical framework of chemistry, complex and interconnected procedures   | <ul style="list-style-type: none"> <li>Compliance with standards, chemical concepts and theories</li> <li>Interconnection</li> </ul> | <ul style="list-style-type: none"> <li>Complex procedures</li> </ul> | <ul style="list-style-type: none"> <li>Enhances thinking</li> <li>Interconnection of synthesis and analysis</li> <li>Concerns: speed, cost and amount of work required, use of hazardous materials, accuracy and reliability</li> </ul> |
| Refined axiological commitments | Evaluations based on standards and compliance with chemical theories, enhances thinking, interconnection of synthesis and analysis, concerns about cost, speed, amount of work, hazardous materials, accuracy/reliability |  |  |   |



procedures are based on the experimental determination of properties of these entities that are due to their chemical composition and are not simply detected without reference to their scientific/chemical content (epistemological commitments). Finally, in compositional analysis, judgements and evaluations are not simply based on the scientific method in general but on chemical concepts and theories (axiological commitments).

Also, based on our data analysis of the microgenetic domain, the title “compositional analysis” captures more effectively the conceptualization of this zone than that of the previous expanded category of “classical analysis”. The title “classical” is mainly associated with classical methods of analysis, thus putting emphasis mainly on the procedures and much less on the entities. The term “compositional” emphasizes the focus on both the components as analytical targets as well as the specific procedures employed for their determination. As evidenced by their responses, students highlight the composition of elements and compounds (atoms, molecules and functional groups), and they often relate the existence of certain components to the properties of elements and compounds

[Part 2] Interviewer: *What do you think causes these properties?*

S2: *...The components that comprise each material determine its properties. And their structure, that is how they are connected... or to particular analytical procedures*

[Part 1] U7: *...White wine, for example, due to its ethanol content, could discolor an acidic solution of  $KMnO_4$ ...*

### Zone: mechanistic analysis

**Ontological commitments.** As established by our secondary data analysis across all genetic domains (Table 14), this zone includes thinking of molecules, atoms and ions that dynamically interact with one another.

The following excerpts are indicative:

[Part 2] Interviewer: *How do you think spectra are produced?*

S2: *...Is there any interaction between carbon atoms and the element with which they are bonded? ...*

[Part 2] Interviewer: *If we could see inside a material, what would we see?*

U2: *...many molecules collide ... great disorder, what we call vibrations, interactions...*

These components have a known and well-defined structure and geometry, as evidenced from the following discourse:

[Part 2] Interviewer: *What do you think to be the cause of these properties?*

U3: *Again, I think it's the way... the structure of the molecules inside, how they are dispersed. In terms of how the molecules themselves are arranged in space and how they are connected. Yes... geometry, in other words. And the atoms themselves, because if we have oxygen and hydroxyl, hydrogen bonds can form. I don't know if density plays a role.*

Interviewer: *What role does density play?*

U3: *Again, consider the material's qualities. But I'm not sure if geometry affects density, so I guess I end up back at geometry again.*

Furthermore, molecules, atoms and ions are composed of dynamically interacting entities (such as protons and electrons).

[Part 2] Interviewer: *What is a material made of?*

U2: *...It all starts with how an atom's electrons are separated into shells and from these shells' bonds can be formed with other atoms. Some atoms are more electronegative and attract electrons...*

As suggested by sociocultural and ontogenetic domains, the above-mentioned entities are determined through the employment of specific instrumental analytical techniques in a laboratory setting. Indeed, students who think of dynamic interactions between entities, inner structure and geometry often opt for an instrumental technique.

[Part 2] Interviewer: *What is a material made of?*

U4: *...From protons, electrons, neutrons... and those are made up of something but I can't remember what... [...]*

Interviewer: *Describe a way you would suggest finding out which material is placed in each container.*

U4: *Yes, okay, so with spectroscopy...*

[Part 2] Interviewer: *If we could see inside a material, what would we see?*

U6: *... How atoms are connected to each other in a molecule. That's what we would see.*

**Table 14** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of mechanistic analysis zone

|                                 | Expanded category   | Zone  |  |   |
|---------------------------------|---|---|--|---|
|                                 |   | Dialogue with microgenetic domain   |  |   |
| Mechanistic analysis            | Dialogue between sociocultural – ontogenetic domains  | YES   | NO   | NEW   |
| Entities                        | Dynamically interacting molecules, atoms, ions composed of dynamically interacting entities (e.g. electrons, protons)   | <ul style="list-style-type: none"> <li>Dynamically interacting molecules, atoms, ions</li> <li>Composed of dynamically interacting entities (electrons, protons)</li> </ul> |  | <ul style="list-style-type: none"> <li>Known structure, geometry</li> </ul> |
| Procedures                      | Isolated instruments in lab   |   | <ul style="list-style-type: none"> <li>Isolated instruments</li> </ul> | <ul style="list-style-type: none"> <li>Specific</li> </ul>                  |
| Refined ontological commitments | Dynamically interacting molecules, atoms, ions with specific structure and geometry composed of dynamically interacting entities (e.g. electrons, protons) and analyzed with specific instrumental procedures |   |  |   |



Interviewer: *What are these atoms made of?*

U6: *Particles such as protons, neutrons, nuclei, electrons. So... ah! We could say that we would also see how they are arranged, we would also see how the electrons are distributed... if I can put it that way... in the space between the bonds, e.g. of some atoms within this compound. [...]*

U6: *Maybe NMR spectra... In fact, it is about nuclear magnetic resonance and one can see the interactions between particles...*

Since we found no references to isolated or coupled instruments in the responses as a whole, we decided that the specific use of the term “isolated” is not required.

**Epistemological commitments.** With respect to the epistemological commitments of this zone, Table 15 displays the results of the dialogic interaction between the microgenetic, sociocultural, and ontogenetic domains.

In line with previous findings, students' answers show that, regarding knowledge construction, this zone is based on certain norms of interpreting analytical signals

[Part 2] U3: *... If I recall properly, the spectra are the result of the number of different carbon atoms that exist... I'm referring to the vibrations of hydrogen and carbon. Let's say we only have one kind of carbon, methyl, which is why we have one peak. So, in fact, the peaks... are determined by the “neighbors” of the carbon we are analyzing...*

in order to determine emergent physicochemical properties as proposed by the sociocultural and ontogenetic domains. These properties are considered emergent because they arise from the interaction of constituent parts of materials and apply to the material as a whole, as demonstrated in the following example:

[Part 2] U2: *... These properties [of the substance] result from the way atoms are bonded to one another and cause the effects we discussed with electron movements, as well as how each interacts with the others...*

We choose to use the more generic phrase “rules of interpretation” instead of the much more precise terms “transformation” and “comparison” of analytical signals. Also, given the theoretical foundation of chemistry and more especially analytical chemistry, one can use the structure and geometry of

molecules, atoms and ions to make deductive predictions and explanations for their properties.

[Part 2] U2: *... The color may also be due to light absorption, and we may see it as yellow or pale yellow, for example. Taste is derived from interactions that occur on our tongue, where we have receptors for various compounds, so I think their three-dimensional structure also plays a very important role...*

**Axiological commitments.** Table 16 shows the outcome of the dialogic interaction between the microgenetic-sociocultural-ontogenetic domains in terms of the zone's axiological commitments.

Contributing to the formation of the axiological commitment, microgenetic domain data suggests that many students base their evaluations on how well the understanding of molecules, atoms and ions as well as the employment of certain processes adhere to the theoretical framework of analytical chemistry and chemistry in general. An implicit reference to the fundamental ideas of analytical chemistry can be found in the following passage:

[Part 2] U6: *... On the other hand, instrumental analysis teaches you how this is done, what equipment and instruments are used, how it is done, and why it is done this way and not another... A new study on classical analytical chemistry should serve as the basis for the development of particular equipment...*

Also, based on students' responses, techniques or procedures often rely on statistical and chemometric notions and they are often characterized as reliable and accurate.

[Part 2] U1: *... I feel NMR provides fairly accurate information...*

[Part 2] U4: *... with the spectra, I can tell exactly what the distinctive groups are and where they are or I can see exactly where everything is with other spectra, such as IR... the spectrum is the most conclusive...*

[Part 2] U9: *... spectra provide more accurate results...*

However, they are complicated due to the numerous chemical concepts that underlie them.

[Part 2] U4: *... I confuse the spectra with one another... there is too much work associated with the spectrum and analyzing it requires a lot of effort...*

**Table 15** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of mechanistic analysis zone

|  | Expanded category   | Zone   |   |  |
|--|---|--|---|--|
|  |   | Dialogue with microgenetic domain  |   |  |
| Mechanistic analysis                                 | Dialogue between sociocultural – ontogenetic domains  | YES  | NO  | NEW  |
| Knowledge construction about entities and procedures | Deductive predictions and explanations within a theoretical framework, emergent physicochemical properties, Transformation and comparison of analytical signals             | <ul style="list-style-type: none"> <li>• Determination of emergent physicochemical properties</li> <li>• Deductive predictions and explanations</li> </ul> | <ul style="list-style-type: none"> <li>• Transformation, comparison of signals</li> </ul> | <ul style="list-style-type: none"> <li>• Rules of interpretation of analytical signals</li> <li>• Theoretical framework of analytical chemistry</li> </ul> |
| Refined epistemological commitments                  | Determination of emergent physicochemical properties, rules of interpretation, deductive predictions and explanations within (analytical) chemistry's theoretical framework | <ul style="list-style-type: none"> <li>• Theoretical framework of chemistry</li> </ul>   |   |  |



**Table 16** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of mechanistic analysis zone

|                                 | Expanded category   | Zone  |   |  |
|---------------------------------|---|---|---|--|
|                                 |   | Dialogue with microgenetic domain   |   |  |
| Mechanistic analysis            | Dialogue between sociocultural – ontogenetic domains  | YES   | NO  | NEW  |
| Evaluations and judgements      | Important – verification tool, accurate, sensitive, non-destructive, fast and with low detection limits, expensive, complicated                     | <ul style="list-style-type: none"> <li>• Accurate yet complicated procedures</li> </ul> | <ul style="list-style-type: none"> <li>• Important, verification tool</li> <li>• Fast</li> <li>• Sensitive</li> <li>• Non-destructive</li> <li>• Low detection limits</li> <li>• Expensive</li> </ul> | <ul style="list-style-type: none"> <li>• Adherence to (analytical) chemistry's theoretical framework</li> <li>• Chemometrics, statistics</li> <li>• Reliability</li> </ul> |
| Refined axiological commitments | Evaluations based on compliance with (analytical) chemistry's theoretical framework and chemometrics/statistics, reliable, accurate yet complicated |   |   |  |

Further evaluations of procedures, such as important, sensitive and fast, are excluded of this zone's axiological commitment because they were not detected in students' replies.

In general, we view mechanistic analysis as a separate zone from compositional analysis rather than a more profound layer of it because mechanistic analysis emphasizes the idea of dynamic interaction between matter's constituent parts. This is evident in all the commitments that differentiate these two ways of thinking. Thus, in mechanistic analysis, entities have a certain chemical structure (and not just a known chemical composition) which results from the dynamic interaction between their components. Procedures are based on these interactions (ontological commitments). Emergent physicochemical properties (due to entities' interactions) are determined by employing these procedures (epistemological commitments). Judgments and evaluations are not just based on chemical concepts and scientific principles in general but on the framework of (analytical) chemistry that has been developed based on the study of interactions between components (axiological commitments).

Also, considering microgenetic domain data, the title "mechanistic analysis" is more representative for the conceptualization of this zone than the title "classical instrumental analysis" of the previous expanded category. This is because the term "instrumental" relates mainly with procedures, while the term "mechanistic" more accurately describes the dynamic interactions of matter's constituent parts at different levels of organization (Machamer *et al.*, 2000; Luisi, 2002; Talanquer, 2018). These interactions determine the properties of matter as well as the related analytical procedures. This way of thinking is particularly clear in the responses of undergraduate students. Secondary school students rarely exhibit this zone, most likely due to their lack of spectroscopic experience.

### Zone: automated analysis

The primary data of the microgenetic domain revealed a way of thinking (entitled automated analysis zone) that was not identified in the previous analysis of secondary data of either the sociocultural or the ontogenetic domains. Thus, for this zone,

the following strategy was adopted: students' answers were first analyzed in a partially inductive manner and then dialogically interacted with data from the sociocultural and ontogenetic domains.

**Ontological commitments.** According to dialogic interaction between data from all three genetic domains (Table 17), those who think about chemical analysis as automated analysis consider that every element and compound with a known or unknown chemical composition may be examined in a lab setting using some instrumental procedure.

This is supported by students' responses, as seen in the following extract:

[Part 1] Interviewer: *What do you think we can analyze?*

U1: *Anything.*

Interviewer: *How do we analyze a material?*

U1: *There are countless instruments for analyzing anything.*

Data from historical and epistemological sources (sociocultural domain) converge on the aforementioned commitment, as they suggest that modern chemical analysis frequently treats entities regardless of their chemical composition, allowing us to examine any entity (*e.g.* Karayannis and Efstathiou, 2012). This form of analysis involves the integration of computers, particularly microcomputers, into nearly any laboratory instrument (Valcarcel, 1992). The results are interpreted directly for practical purposes, such as determining specific elements and compounds with instruments (Jin *et al.*, 2015) or unknown elements and compounds with more advanced instrumentation in non-target analysis (Pehlivanoglu *et al.*, 2024).

Concerning the ontogenetic domain, the majority of students' alternative ideas originate from a non-structured perspective on instrumental analysis principles and processes (Doménech-Carbó *et al.*, 2009). This is partially due to the fact that teaching emphasizes how to employ particular analytical techniques rather than fostering a comprehensive understanding of chemical analysis in terms of both entities and procedures. Even though this approach is a large part of chemical analysis practice often employed by experts, it can lead to a fragmented perception of the discipline, where students view



**Table 17** Dialogic interaction between data from all three genetic domains leading to the refinement of the ontological commitments of automated analysis zone

| Automated analysis              | Microgenetic domain  | Zone  |    |  |
|---------------------------------|--|---|----|--|
|                                 |  | Dialogue with sociocultural and ontogenetic domains   |    |  |
|                                 |  | YES   | NO | NEW  |
| Entities                        | Any  | <ul style="list-style-type: none"> <li>Entities are treated regardless of chemical composition</li> </ul> |    | <ul style="list-style-type: none"> <li>Target or non-target analysis (known or unknown chemical elements and compounds)</li> </ul> |
| Procedures                      | Instrumental   | <ul style="list-style-type: none"> <li>Instruments</li> </ul>   |    | <ul style="list-style-type: none"> <li>Any method or set of methods including instruments</li> </ul>                               |
| Refined ontological commitments | Every element and compound with known or unknown chemical composition analyzed using some instrumental procedure |   |    |  |

chemical analysis as a collection of methods rather than a unified field with underlying principles and problem-solving strategies (Enke, 2001; Adams and Adriaens, 2020).

Thus, incorporating data from all three genetic domains, those who think about chemical analysis as automated analysis are ontologically devoted to the idea that, regardless of their known or unknown chemical composition, every element or compound could be analyzed employing any procedures including any instrument in a laboratory.

**Epistemological commitments.** Regarding this zone's epistemological commitments, Table 18 displays the results of the dialogic interaction between the microgenetic, sociocultural and ontogenetic domains.

Their answers reveal that students think that chemical analysis relies on a set of measurements and determinations gathered by specific instruments in an automated manner heavily relying on technology

[Part 2] S3: ...with the use of technology, the instrument practically completes the task without human intervention...

[Part 2] U1: ...everything is done by a computer...

[Part 2] Interviewer: If you had used information from this table [spectra – Table E (SI)], how would your answer change?

U5: ... results will be made available in an automated way... and mostly by comparing the results to previously known analytical results.

[Part 2] Interviewer: How did you think in order to find out which component exists in a specific material?

S2: ...the specific spectrum that would be produced... I would have a list of the spectrum belonging to each chemical compound and I would match them up...

[Part 2] Interviewer: How did you think of the way in which you will determine which component exists in a specific material?

U5: ...with analytical methods, i.e. chromatography or any other analytical method, potentiometry... which I may have from the bibliography, and match, and in case there are many things that characterize something, I separate them from each other to understand what I have, if I can...

There is a difference between the usage of these data and the real understanding of methods gathering them, because of the limited knowledge and comprehension of theory. This is evident in the examples that follow: while the student S5 acknowledges the use of spectra, he is unsure of the precise meaning of the numbers on the spectrum. Also, he acknowledges that while spectra are helpful, nobody knows exactly what it is being done.

[Part 2] S5: ...I assume they gather measurements and determine how much of each substance there is, but I'm not sure what the numbers are or why they are here... Only with this [spectra], we won't have truly comprehended it or learnt what we have done. We'll measure it, all right, but what will we think about what we have done? What do we really understand? ...

Student S1 thinks she can use results from spectra without, however, being able to relate what the spectrum shows (in this case, chemical structure) to other information and knowledge (in this case, color or pH).

[Part 2] S1: ...With spectra, you can find the number of atoms and how many there are and what they are made of, but you cannot see properties such as color, perhaps, or pH, let's say...

Indeed, concerning the sociocultural domain, the integration of technology, particularly computers and microcomputers

**Table 18** Dialogic interaction between data from all three genetic domains leading to the refinement of the epistemological commitments of automated analysis zone

| Automated analysis                                   | Microgenetic domain  | Zone  |  |  |
|--|--|---|--|--|
|  |  | Dialogue with sociocultural and ontogenetic domains   |  |  |
|  |  | YES   | NO   | NEW  |
| Knowledge construction about entities and procedures | Automation, technology, comparison with other results, limited knowledge and understanding of theory   | <ul style="list-style-type: none"> <li>Automation/technology</li> <li>Comparison</li> <li>Limited use of theory and models</li> </ul> | <ul style="list-style-type: none"> <li></li> </ul> | <ul style="list-style-type: none"> <li>Libraries for comparison</li> </ul> |
| Refined epistemological commitments                  | Comparison with already known results of analysis (e.g. libraries), automation and technology, limited knowledge and understanding of (analytical) chemistry's theoretical background and models |   |  |  |



which enhance automation (Karayannis and Efstathiou, 2012) can be greatly beneficial in knowledge construction as well. Nonetheless, it is supported that the process of the development of chemical theories changed as a result of instrumentation, with a focus on rules for converting signals into chemical information (Schummer, 2002; Slater, 2002). Additionally important for substance identification, particularly after 2000, is the comparison with previously known analysis results (e.g., mass spectral libraries) (Stein, 2012; Milman and Zhurkovich, 2016).

This relates to a key theme in the history and philosophy of chemical analysis, namely *naïve instrumentalism*, where instruments are treated as “black boxes” that reliably produce results without requiring chemists to understand the underlying scientific principles. This approach has enabled chemists to operate complex instruments by following established procedures or simplified theoretical frameworks, often provided in textbooks. As a result, they can interpret data without deep knowledge of the science behind the instrumentation, which parallels the use of those working in industry who use instruments without understanding their inner workings. This development has facilitated the widespread adoption of instrumental methods but also raises questions about the depth of understanding and critical engagement with the data produced (Wolfgong, 2016).

Along with naïve instrumentalism, *non-model-based reasoning* in chemical analysis also shares a practical orientation and a reliance on instrumentation for direct measurement. However, while naïve instrumentalism may involve a lack of concern for deeper theoretical justification, non-model-based reasoning is characterized by the absence of explicit models, often requiring advanced expertise for data interpretation, especially in nontarget analyses (Hughes, 2009; Jin *et al.*, 2015; Wolfgong, 2016; Pehlivanoglu *et al.*, 2024). While both approaches can be effective in achieving analytical goals, non-model-based reasoning may demand more collaboration among chemists and other scientists due to the challenges of working without established models (Pehlivanoglu *et al.*, 2024).

Our finding from the microgenetic domain that information about compounds arises automatically and mostly through comparisons is also supported by the ontogenetic domain. Specifically, data on students' alternative conceptions suggest that learners frequently advocate for automatic data analysis that ignores alternatives (Doménech-Carbó *et al.*, 2010) and they think about chemical analysis results without fully understanding (analytical) chemistry concepts and without directly linking them to the physicochemical properties of compounds (Karayannis and Efstathiou, 2012). Furthermore, during analysis, the operation of the equipment and the theoretical basis of the instrumental approach are often viewed by students as secondary or insignificant. As a result, instruments seem as mysterious black boxes that just provide results (Doménech-Carbó *et al.*, 2010). Additionally, students believe that the primary goal is to learn how to operate specific instruments or perform particular procedures, rather than to understand the underlying analytical concepts (Enke, 2001).

Therefore, we propose that the epistemological commitment of this zone, which incorporates data from all three domains in a dialogic way, states that, when considering chemical analysis as automated analysis, people build their knowledge by comparing results to previously known analytical results while heavily relying on technology and automation. There is limited knowledge and comprehension of the theoretical foundations and models of (analytical) chemistry.

**Axiological commitments.** In terms of the zone's axiological commitments, Table 19 displays the results of the dialogic interaction between the microgenetic, sociocultural, and ontogenetic domains.

From an axiological aspect, procedures are commonly evaluated by participants as certain, precise and accurate.

[Part 2] Interviewer: *What about spectra?*

S4: *I think we would be sure.*

Interviewer: *What makes you say that?*

S4: *I think it's absolutely certain, as it appears in the picture [Table E, SI]. . . I don't know what it is, actually. But I think it will be something certain.*

[Part 2] S7: *. . . I feel that the spectra are more accurate; that is, you will test them and get exactly what you want. . .*

[Part 2] U4: *. . . If we have a pH meter. . . I guess it offers precision. . .*

Some students believe that we can learn everything we want about substances in detail, as shown in the following example:

[Part 2] S6: *. . . [using spectra] we can analyze the material in great detail because we get to know its composition, if they are branched. . . For us to determine everything else, we first need to carry out this [spectra]. . .*

But others are concerned about the type of analysis outcomes because information on entities is only structural and details about substances' properties cannot be directly obtained, for instance:

[Part 2] S1: *. . . using spectra, you cannot discern properties like color, pH, or solubility. . .*

Additionally, procedures are perceived as complex, boring and uninteresting, hard to comprehend and theoretical in the sense that they lack hands-on activities.

[Part 2] S9: *. . . I didn't use the spectra because they confuse me. . .*

[Part 2] U2: *. . . simply providing you with spectra or using a computer. . . in my opinion, none of these options is particularly engaging and interactive. . .*

Furthermore, some individuals voice worries regarding the expense and speed of procedures.

[Part 2] S7: *Concerning spectra, you probably need machines to create them; so, money is required and not everyone may be able to provide it.*

[Part 2] U2: *. . . disadvantages perhaps financially, because you need to maintain a machine. . .*

[Part 2] U5: *. . . and the spectra may be fast. . . we measure in seconds. . .*

[Part 2] Interviewer: *Could this approach [spectra] have disadvantages compared to the one you had suggested before [reactions]?*



**Table 19** Dialogic interaction between data from all three genetic domains leading to the refinement of the axiological commitments of automated analysis zone

| Automated analysis              | Microgenetic domain   | Zone  |  |   |
|---------------------------------|---|---|--|---|
|                                 |   | Dialogue with sociocultural and ontogenetic domains   |  |   |
|                                 |   | YES   | NO   | NEW   |
| Evaluations and judgements      | Certain, accurate, precise, concerns of the information obtained/cost/speed, boring, complex, hard to comprehend and theoretical  | <ul style="list-style-type: none"> <li>Concerns about cost</li> <li>Precise</li> </ul>                                  | <ul style="list-style-type: none"> <li>Boring</li> </ul> | <ul style="list-style-type: none"> <li>Sensitive</li> <li>Compromises (concerns)</li> </ul> |
| Refined axiological commitments | Error-free, certain, accurate procedures, difficult to understand/theoretical/complicated entities and procedures, concerns about speed as well as cost and availability of equipment | <ul style="list-style-type: none"> <li>Error-free</li> <li>Difficult to understand, complicated, theoretical</li> </ul> |  |   |

S6: *The downside is that it [spectra] takes more time...*

Even though in the sociocultural domain it is argued the compromises are made between sensitivity, precision and cost with the purpose of minimizing analytical error (Karayannis and Efstathiou, 2012), students are ignorant of it (Doménech-Carbó *et al.*, 2009; Karayannis and Efstathiou, 2012). Furthermore, a pseudo-empiricist assumption of scientific practice prevails as they frequently have a mental model that includes an error-free belief in data obtained from instruments and experimentation in general (Doménech-Carbó *et al.*, 2009). Most of the times, equipment is thought of as a precise, independent and semi-automated device (Doménech-Carbó *et al.*, 2010). As already mentioned, both analytical chemistry and metrological terms are considered hard to understand and complicated (Doménech-Carbó *et al.*, 2010; Karayannis and Efstathiou, 2012).

Therefore, considering data from the microgenetic as well as the sociocultural and ontogenetic domains, the axiological commitment of the automated analysis zone appears in evaluations and judgments about procedures that are thought to be error-free, certain and always accurate. Furthermore, entities along with procedures are considered theoretical and overly complex, making them difficult for people to understand and thus constraining their thinking. Concerns about speed as well as the cost and the availability of equipment are frequently raised.

### Overview

Overall, six zones constitute the proposed conceptual profile of chemical analysis. Table 20 presents a synoptic report of the ontological, epistemological and axiological commitments that establish and stabilize these six zones.

Recently, the concurrent examination of the sociocultural and ontogenetic domains led to the proposal of a way of thinking about chemical analysis as a “contemporary tool for society” (Mavridi *et al.*, 2025). In the light of this expanded category, chemical analysis deals with entities that are typically associated with social, economic or environmental issues and are determined by linear methods employing coupled instruments in the laboratory or in the field. Regarding the epistemological commitment, large data about entities and

analytical procedures, the use of chemometrics, the integration of microcomputers into all instruments and collaboration among related scientific disciplines like physics, mathematics, informatics and so on are all related to knowledge construction about chemical analysis. Also, the range of perspectives (positive, neutral and negative) that take into account not only the intricacy of chemical analysis itself but also its interactions with society, economy and environment provide the axiological commitment of this way of thinking. To reduce analytical error, tradeoffs are made between sensitivity, precision and analysis cost. A false empiricist assumption can occasionally prevail due to the emphasis on instruments and experimentation, which reduces the role of significance in data interpretation.

However, nearly every participant commented that, while information about how entities relate to social, economic and environmental issues may be valuable as broad knowledge, it is completely useless when it comes to chemical analysis. It seems that students’ choice of analytical methods and procedures is unaffected by societal expectations resulting from various real-world situations (Doménech-Carbó *et al.*, 2010), even though the social dimension of chemical analysis is largely important. Here are some notable extracts from high school and university student comments about Table F (SI), where the relevant information was presented.

[Part 2] S3: *...The advantages of Table F (SI) include a clearer understanding of how substances benefit us, what we do with them and what they are related to. The downside is that they do not help so much in this particular experiment...*

[Part 2] S9: *...I don't think it [Table F (SI)] helps me in any particular way...*

[Part 2] U3: *...I believe we should first determine what substance we have in our hands before deciding where we can use it. That is why I did not use it [Table F (SI)] throughout the separation...*

[Part 2] U4: *...here [Table F (SI)] we basically have information that does not relate to the laboratory setting, so it's not useful to me...*

[Part 2] U7: *...The truth is that I personally don't see any particular relationship. I mean, if I needed a table to use from all of these, this [Table F (SI)] would probably be the last one...*



Table 20 Proposed zones of a conceptual profile model of chemical analysis

| Zone                   | Commitments  |   |  |
|------------------------|--|---|--|
|                        | Ontological  | Epistemological   | Axiological  |
| Everyday analysis      | Materials as <b>stuff</b> or <b>objects</b> analyzed with simple procedures employing <b>human senses</b> , not necessarily in laboratories  | Use of senses – observation of <b>explicit</b> or <b>object-related</b> properties, functions and origin, independently of theory   | Only <b>simple</b> and <b>useful</b> materials are analyzed with fast, easy, simple, yet subjective, inaccurate, dangerous procedures  |
| Alchemical analysis    | Materials having an <b>essence</b> analyzed with procedures employing human senses or simple experiments   | Observation of <b>essential</b> and <b>additive</b> properties, partially using or independently of relevant theory   | <b>Fusing</b> domains of experience-knowledge  |
| Empirical analysis     | <b>Elements</b> and <b>compounds</b> as <b>components</b> of mixtures or pure materials analyzed with basic <b>experimental</b> procedures   | Observation and detection of <b>emergent physical and chemical</b> properties, operational categorization, vaguely based on theory  | Evaluations based on compliance with <b>theory</b> and <b>scientific method</b> , concerns about easiness, objectivity, accuracy   |
| Compositional analysis | Elements and compounds with specific chemical <b>composition (molecules, functional groups, atoms)</b> analyzed with classical experimental procedures   | Determination of <b>fixed physical and chemical</b> properties, <b>structure-property relationships</b> , compositional categorization, based on chemical theories and concepts                                 | Evaluations based on <b>standards</b> and compliance with <b>chemical theories</b> , enhances thinking, interconnection of synthesis and analysis, concerns about cost, speed, amount of work, hazardous materials, accuracy/reliability |
| Mechanistic analysis   | Dynamically <b>interacting</b> molecules, atoms, ions with <b>specific structure and geometry</b> composed of dynamically <b>interacting</b> entities ( <i>e.g.</i> electrons, protons) and analyzed with specific instrumental procedures | Determination of <b>emergent physicochemical</b> properties, rules of interpretation, deductive predictions and explanations within (analytical) chemistry's theoretical framework                              | Evaluations based on compliance with <b>(analytical) chemistry's theoretical framework</b> and chemometrics/statistics, reliable, accurate yet complicated   |
| Automated analysis     | Every element and compound with known or unknown chemical composition analyzed using some instrumental procedure   | Comparison with <b>already known results</b> of analysis ( <i>e.g.</i> libraries), automation and technology, limited knowledge and understanding of (analytical) chemistry's theoretical background and models | Error-free, certain, accurate procedures, <b>difficult</b> to understand/theoretical/complicated entities and procedures, concerns about speed as well as cost and availability of equipment   |

[Part 2] U8: ...*I'm not sure where this [Table F (SI)] could be relevant to the analysis.*...

Additionally, students occasionally express that they do not fully comprehend the information about societal aspects of various substances and the related analytical procedures,

[Part 2] S1: ...*For example, these [Table F, SI], even if they are about society and all, I don't have them... at school, let's say, we haven't really discussed these.*...

which is in line with research suggesting that students do not always understand entities, concepts or procedures related to social needs, such as environmental analysis, quality assessments in industry, *etc.* (Doménech-Carbó *et al.*, 2009). Also, as previously noted, we did not find any references to either coupled or isolated instruments in the responses as a whole. Therefore, we argue that the way of thinking (expanded category) about chemical analysis as “contemporary tool for society” is not compatible with our proposed conceptual profile model of chemical analysis.

The reader should bear in mind that the zones were established based on the differentiation of the ontological, epistemological and axiological commitments rather than the complete replacement of entities or procedures by others. Thus, even if the boundaries of zones of our proposed model may not always be as clear (Vershinin and Zolotov, 2009), zones should be seen in light of their respective commitments, which together establish, stabilize and differentiate a specific way of thinking from another. Any overlap between the zones highlights the dynamic character of the conceptual profile theoretical framework (Liu and Lesniak, 2006). Details on the formation and thorough description of the commitments of

the expanded categories of thinking that interact with micro-genetic data in the current study have been documented in the first part of this research (Mavridi *et al.*, 2025) and are not presented in this article.

We should keep in mind that chemical analysis is a complex concept that involves both material entities (the targets/end-points of analysis) and analytical procedures (Chi *et al.*, 1994; Klein and Ragland, 2014; Seviaan and Talanquer, 2014). Therefore, knowledge of materials and chemical substances has always been connected to chemical analysis. The sociocultural domain findings (Mavridi *et al.*, 2025) make clear that the current understanding of matter in a particular historical period determines the answer to the fundamental question of analysis, “*What is the world and matter around us made of?*” (Weisberg *et al.*, 2019), namely principles, elements, atoms, ions, parts of molecules or molecules, which are the targets/endpoints of analysis (Klein and Ragland, 2014; Zolotov, 2020).

The understanding of matter is related to questions about chemical identity in the ontogenetic domain, like “*What types of matter are there?*” and “*What cues are used to differentiate matter types?*” (Seviaan and Talanquer, 2014). Through the employment of certain analytical procedures, chemical analysis provides information about chemical composition; in particular, qualitative analysis suggests the chemical identity of the substances in a sample based on the differentiation of substances at least by one property (Ngai and Seviaan, 2017; Talanquer, 2019).

The aforementioned connection between other concepts and that of chemical analysis should be kept in mind when studying the proposed conceptual profile model. Nevertheless,



one should not overlook the conceptual meaning of chemical analysis *per se*, which essentially lies in complex bodies dissolving into their components (Simon, 2002).

There are two limitations of our work related to the overall data analysis approach as acknowledged by its founders (Mortimer *et al.*, 2014a). First, a preliminary classification of the various ways of thinking was suggested as a result of our reviewing of philosophical, historical and alternative ideas sources (Mavridi *et al.*, 2025). After contributing to analyzing the students' comments, these categories were further refined, and zones were then established. Primary empirical data, however, were in some cases more detailed than the categorization derived from the ontogenetic and sociocultural, thus there is a possibility of bias for the interpretation of these data.

Second, for the automated analysis zone, the study of the microgenetic domain initially established this zone's commitments, which were subsequently refined by the sociocultural and ontogenetic domains. The methodology of developing a conceptual profile model, as proposed by the pioneers of this methodological framework, is congruent with the proposal of a new zone that begins with microgenetic data. Additionally, it demonstrates the dialogical nature of our data analysis process by interactively reviewing all data sources. However, there is a possibility of a poor categorization derived from primary data. In each of these cases, we sought to reduce the impact of these risks by ongoing dialogue between data from each of the three genetic domains (Mortimer *et al.*, 2014a).

## Conclusions

In conclusion, this study proposes the zones of a conceptual profile model of chemical analysis based on the dialogic interaction of microgenetic domain data with sociocultural and ontogenetic domain data. In particular, the previously proposed expanded categories of ways of thinking about chemical analysis that emerged from the study of historical and epistemological sources as well as students' alternative conceptions (Mavridi *et al.*, 2025), were used as a coding framework for the analysis of primary data obtained from secondary school and university students' responses to interview questions about chemical analysis.

In response to our research questions, the ontological, epistemological and axiological commitments that differentiate and stabilize each of five expanded categories of ways of thinking about chemical analysis previously proposed by the sociocultural and ontogenetic domains: everyday analysis, alchemical analysis, empirical analysis, classical analysis and classical instrumental analysis were enriched and refined through the dialogic integration of microgenetic domain data. Thus, these categories evolved to five zones, as follows: everyday analysis, alchemical analysis, empirical analysis, compositional analysis and mechanistic analysis respectively. The dialectic discussion between primary data from microgenetic domain and secondary data from sociocultural and ontogenetic domains revealed one more zone, the automated analysis zone.

The results of our study cannot be generalized due to the qualitative nature of our research. Nonetheless, some insightful remarks and educational implications could be shared.

To begin with, the variety of ways of thinking, *i.e.*, the zones we detected in different people and in the same individuals at different moments throughout the interview, is remarkable: all zones were found in both secondary school and university students. Furthermore, empirical analysis is particularly prevalent among secondary school students, while compositional and mechanistic analysis appear more frequently among university students. This is not unexpected since secondary school students, unlike university undergrads, do not encounter much spectroscopy during their study.

As has been observed in earlier studies pertaining to conceptual profiles (Mortimer *et al.*, 2014a; da Silva Costa and dos Santos, 2022), the same individual demonstrates a diversity of ways of thinking, or zones: in most participants four to five distinct zones were identified. This means that even if they possess, for instance, the zone pertaining to the dynamic interactions between components, namely the mechanistic analysis zone, in some cases they did not feel the need to apply it and instead resorted to simple, everyday organoleptic procedures, namely the everyday analysis zone. This is true for both secondary school and university students. Similarly, it was noted that in the more general questions about chemical analysis, participants employed certain zones on their own initiative and others only when the interviewer encouraged them to do so. It appears that the nature/type and specifications of each question either encouraged or discouraged participants from using a certain zone (Mortimer *et al.*, 2014b).

With regard to chemistry education the above mentioned remarks imply that that irrespective of level (secondary or tertiary), educational practices should be oriented not only toward the development of particular ways of thinking about concepts (those that students do not yet have according to their grade level) (Mortimer *et al.*, 2012), but also toward awareness of the zones so that students realize the contexts in which each different way of thinking is appropriate (El-Hani *et al.*, 2015; Mortimer *et al.*, 2014b; Aguiar *et al.*, 2018). Additionally, at the very end of the interview, several participants expressed positive feelings for the entire process and considered the discussion to be engaging. This suggests that students may respond favorably to educational approaches that incorporate diverse perspectives and ways of thinking about scientific concepts.

Further research might examine how profile zone distribution varies in different cultural or social settings as well as investigate the social dimensions of chemical analysis in students' thinking and the reasons why it appears to lack appropriate meaning for them. Additionally, one should keep in mind that the proposed conceptual profile model only includes the various ways of thinking that emerged from the interaction between the data of all three genetic domains. This means that this model can be improved to serve as a dynamic and useful asset for both researchers in chemistry and science education and teachers to investigate the cognitive aspect in students'



discourses while they engage on chemical analysis tasks in the classroom.

Overall, the employment of a conceptual profile model of chemical analysis is expected to provide a solid foundation for a more thorough comprehension of students' perspectives on chemical analysis thus further enhancing the development of innovative, research-based instructional strategies aiming at improving chemistry education.

## Author contributions

Conceptualization, M. M., K. S., D. K.; methodology, M. M., K. S., D. K.; formal analysis, M. M., K. S., D. K.; writing – original draft preparation, M. M., K. S.; writing – review & editing, M. M., K. S., D. K.; supervision, D. K. All authors have read and agreed to the final version of the manuscript.

## Conflicts of interest

The authors declare no conflict of interest.

## Data availability

Data of this article cannot be made available due to ethical confidentiality requirements.

Supplementary information (SI) is available. See DOI: <https://doi.org/10.1039/d5rp00441a>.

## Ethical considerations

All aspects concerning the ethical requirements for the conduct of this research have been approved by the Ethics committee of Ionian University.

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