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Supporting Chemistry Students' Understanding of Zeolites with Mixed Reality

An Exploratory Design Study

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Author note

The target audiences of this paper are educational designers and chemistry teachers. Part of the paper may be published in journals such as the Journal of Science Education and Technology.

Abstract

Mixed reality technology is likely beneficial to chemistry education, yet little research has been done on the topic. In this study, I explore considerations in the design of a mixed reality tool that supports chemistry students' understanding of zeolites. The design was informed by expert meetings, an expert workshop, concept mapping and rapid prototyping with mixed reality technologies available online. The design was subsequently evaluated via walk-throughs and semi-structured interviews with a chemistry teacher and an educational designer. The findings suggest that, at least for the secondary school level, it is easier to identify learning processes than subject areas that may benefit from mixed reality. Micro-macro-meso level reasoning about carbon cracking with zeolites was found to be a viable topic. Five choices that must be made in the design process are identified and described. Although the findings are not exhaustive, they may serve as an example or starting point for educational designers and chemistry teachers who are designing a mixed reality tool. Recommendations are given about how to select a chemistry subject area or learning process and a mixed reality platform. Outsourcing the development process is only recommended after several prototypes have been developed and evaluated.

Keywords: mixed reality, mixed reality design, secondary school chemistry, micro-macro-meso level reasoning, zeolites

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Mixed reality technology is three-dimensional by nature and can be immersive and interactive. Augmented reality, for example, can bring the two-dimensional image of a dinosaur to life as a three-dimensional object. Virtual reality offers immersion in places you otherwise would not be able to go, such as the planet Mars or deep under the ocean. Mixed reality is therefore thought to be suitable for educational purposes (Akcayir & Akcayir, 2017; Birt & Cowling, 2017; Radu, 2014). However, because the technology is still emerging, it is unclear how mixed reality can be designed to support students most effectively. The added value of mixed reality to specific school subjects such as chemistry remains largely unaddressed (Maas & Hughes, 2020).

Mixed reality may be especially suited for chemistry education. Chemists generally seek to understand and explain natural phenomena such as electricity, fire, and magnetism. The concepts they use in their explanations are exceedingly small and invisible. Molecules, for example, are invisible to the naked eye. To gain an understanding of these invisible concepts, magnified physical models can be used. Yet the fabrication of physical models is costly and time-consuming. Additionally, physical models are often static structures that are difficult to manipulate and interact with (Chen, 2006).

Mixed reality is likely a valid and valuable alternative to physical models. In mathematics education, researchers found that augmented reality geometric models had the same learning effects and the same size learning effects as physical geometric models (Gün & Atasoy, 2017; Lin et al., 2015). If this holds true for augmented reality models in chemistry education, it will significantly reduce fabrication costs and time.

There is another argument for mixed reality being suitable for chemistry education. Chemistry students often find it difficult to translate a two-dimensional textbook image to three-dimensional mental image (Harle & Towns, 2010; Wu & Shah, 2004). When they do successfully form a three-dimensional mental image, students may have trouble with rotationand reflection transformations. Mixed reality could likely support these students by projecting a three-dimensional overlay onto a textbook image or into a virtual reality. Students would then be able to manually manipulate and transform the three-dimensional image. This would remove the need for complex mental rotating and transforming and it would support students in constructing a correct three-dimensional mental model.

As stated previously, the development of mixed reality tools for the chemistry classroom is largely uncharted territory. That is why, in this study, I explore possible considerations in the design process of a mixed reality tool. I identify chemistry subject areas and usage scenarios that could benefit from mixed reality technology. One of these examples is developed and studied further, with the goal to provide actionable knowledge. The knowledge may be used for two purposes. First, it will serve as preliminary research in the design process of a mixed reality tool made for the Freudenthal Institute by mixed reality designers. Second, it may be used by both chemistry teachers and educational designers to help guide their own mixed reality design and development process.

Theoretical background

Mixed reality technology

Augmented reality and virtual reality are three-dimensional overlays to reality that are generated by computers. In augmented reality, students simultaneously view the augmented reality and the real world. In virtual reality, students view only the virtual reality and not the real world. Reality and virtual reality lie at opposite ends of the Reality-Virtuality continuum (see Figure 1). The overlapping concept 'mixed reality' encompasses the entire Reality-Virtuality continuum. In this study, the concept mixed reality indicates either augmented reality or virtual reality or both.

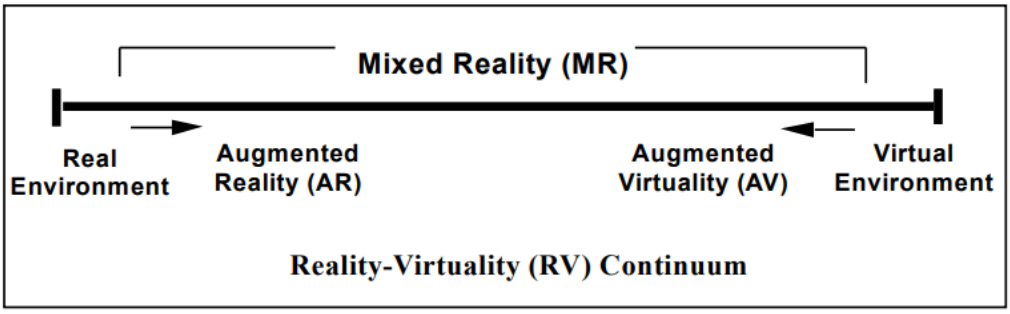

Figure 1. Mixed Reality: a continuum of reality and virtuality. Note: reprinted from 'Augmented Reality: A class of displays on the reality-virtuality continuum,' by P. Milgram, H. Takemura, A. Utsumi and F. Kishino, 1994, *Telemanipulator and Telepresence Technologies, 2351*, p. 283.

Augmented reality and virtual reality lie on different points of the Reality-Virtuality continuum and as a result both share and differ in characteristics. Virtual reality is *immersive*, whilst augmented reality is generally not. According to Dede (2009), immersion may be defined as "the subjective impression that one is participating in a comprehensive, realistic experience" (p. 66). In virtual reality students are completely submerged into a virtual environment with sounds, images and sensations separate from reality. In augmented reality, students similarly engage with a virtual object. Yet even though the object 'feels real', the experience is less compelling, as students remain aware of their actual surroundings at all times (Chen, 2006; Maas & Hughes, 2020).

Both virtual and augmented reality can be described as facilitating a certain amount of *interaction*. Interaction is here defined as the ability to manipulate virtual objects or the virtual environment through body- and limb movement. According to Radu (2014), students' conceptual understanding of content is enhanced by the encoding of tactile information. Additionally, interaction increases the feeling of being present and motivates students to want to learn more (Dawley & Dede, 2014). Until recently interaction was only possible with heavy and expensive head-mounted displays. This made interactional mixed reality impractical for the classroom (Akcayir & Akcayir, 2017). However, currently even smartphones are able to facilitate interactive mixed reality (Jensen & Konradsen, 2018).

A characteristic often used to describe virtual reality is by its *degrees of freedom* (DoF) it has. In virtual reality, students interact with the virtual environment by moving their head. A device, such as a smartphone or a head-mounted display, tracks these movements and adjusts the virtual environment accordingly. In 1999, the multinational HP Inc. patented a movement tracker with six DoF (U.S. Patent No. 64178366B). They described the first three DoF as "left-right, forward-backward and up-down movement, also known as X, Y, Z translational position". The next three DoF are described as "three angular or orientation parameters, i.e., roll, pitch, and yaw" (p. 7).

Certain mixed reality technologies have more DoF than others. Stationary virtual reality with 3DoF offers only left-right, up-down and sometimes forward-backward movement. Room-scale virtual reality with 6DoF also offers roll, pitch, and yaw movement. Chandrasekera et al. (2019) found that virtual reality with 6DoF provides a higher sense of presence than 3DoF. The DoF also determine the amount of interaction that can take place with the virtual environmental, and thus the manner in which learning takes place.

Learning effects of mixed reality

Previous research showed that mixed reality can have a positive effect on learning outcomes in the affective and conative domain (Akcayir &Akcayir 2017; Radu, 2014). Augmented reality increased student engagement, interest, enjoyment and satisfaction in comparison to traditional classroom instruction (Maas & Hughes, 2020). The acquisition of skills such as juggling a ball or flying a plane increased when practiced in realistic virtual reality scenarios (Jensen & Konradsen).

The effect of mixed reality on learning outcomes in the cognitive domain is less straightforward (Maas & Hughes, 2020). Studies by Furio et al. (2015) and Chen and Wang (2015) showed that students perform better on tests when they receive AR-embedded instruction instead of traditional classroom instruction. On the other hand, Chang et al. (2010) found no significant learning improvements in middle school students using mixed reality. Echeverria et al. (2012) showed no significant learning improvement when using an augmented reality environment either. As a result, the effect of mixed reality on cognitive learning outcomes remains relatively unclear. That is why this study will focus on designing a mixed reality tool that will support a learning outcome from the cognitive domain: the understanding of a (to be specified) chemistry topic.

Design-based research with rapid prototyping

The research strategy of this study originates from the educational design research framework by Plomp (2013) and Bakker (2018). Research done within this framework intends to generate actionable knowledge by studying the potential of new technology. The developmental phase of the framework consists of iterative cycles wherein prototype interventions are developed and evaluated formatively. Nieveen and Folmer (2013) describe research instruments that are typically used to evaluate prototypes formatively. These educational design research instruments, such as expert meetings and walk-throughs, will be used in this study.

In addition, rapid prototyping is used to assess the quality of prototypes formatively. The concept of rapid prototyping stems from engineering and manufacturing. Meier and Miller (2016) described that the approach may also be used to quickly and cheaply design instruction material. They state that rapid prototyping has the goal of identifying problems before too much time and money is invested. In this study, I will use rapid prototyping to test isolated features of an envisioned prototype. This allows me to evaluate features of mixed reality platforms without investing too much time in the design of a complete prototype.

Research Question

Stebbins (2001) stated about exploratory research, "to understand well any phenomenon, it is necessary to start by looking at it in broad, nonspecialized terms" (p. 8). A researcher should be flexible and able to change direction when new insights emerge. That is why the research question in this study is broad and open-ended. The only limit to the scope of the research is the focus on a learning effect in the cognitive domain: understanding. This is formulated as the following research question: *What are considerations in the design of a Mixed Reality prototype that supports chemistry students' understanding?*

Method

In this exploratory design-based research study, a mixed reality prototype was developed and evaluated. The final prototype consisted of a *storyboard* for a mixed reality tool, and a *three-dimensional environment* corresponding with part of the storyboard. Prototype development was informed by expert meetings, an expert workshop, chemistry subject study materials, concept mapping, and rapid prototyping with various mixed reality technologies available online. Prototype evaluation was informed by expert walk-throughs of the prototype, semi-structured interviews, and a questionnaire.

Participants and privacy

Participants were found through contacts of the Freudenthal Institute. The experts consulted in the developmental stage of the study are not referred to by name to ensure their anonymity. The genderless pronoun 'they' is used instead of 'she' or 'he'. Only their general fields of expertise are mentioned, their exact job titles are not. The interviewees in the evaluative stage of the study were given the option to be anonymized yet declined. All participants were fully informed of the aims of the study. The walkthroughs and semi-structured interviews were recorded and transcribed, after which the audio-recordings were destroyed. The transcriptions are saved (solely) on a secure University Utrecht server by the supervisor of this study: dr. H.E.K. Matimba. Field notes and other study materials are destroyed on conclusion of the study.

Procedure & data collection

Development of the storyboard

An expert workshop with a group of secondary school chemistry teachers and chemistry teachers in training (n=26), who previously attended a U-talent lecture about virtual reality in *chemistry education*. The participants were asked to create a lesson plan with virtual reality that would be relevant to their own teaching practice. I observed the workshop activities, made field notes, asked the experts for further explanation when deemed necessary and gathered the lesson plans after the workshop had finished. The findings from the expert workshop and the resulting choices made in the design process were evaluated with a different group of secondary school chemistry teachers and chemistry teachers in training in the evaluative part of the study.

Two expert meetings (n=1, n=2) with a university professor of catalysis and a university professor of inorganic chemistry. During the meetings ideas and possible scenarios for the mixed reality tool were explored. Early prototypes were designed on paper and evaluated through e-mail conversations with the experts. Based on the meetings, the chemistry subject carbon cracking with zeolites was chosen as the topic of the mixed reality tool. A brief explanation about the topic can be found in Appendix A.

Chemistry study materials about the chosen topic were gathered online and through contacts of the Freudenthal Institute. These materials were used to inventory the concepts commonly used in relation to carbon cracking with zeolites. I visualized the relevant concepts and their relation to each other in a concept map (Appendix B). This concept map was used to guide the development of the storyboard.

Development of the three-dimensional environment

An expert meeting with a researcher currently designing and evaluating virtual reality lesson materials in the context of lesson study for the chemistry classroom. This meeting focused on the rationale behind the expert's choice for a specific virtual reality technology.

An expert meeting with an artificial intelligence researcher currently investigating the efficacy of mixed reality in general education. This meeting focused on the possibilities and limitations of different mixed realities technologies in general education.

Rapid prototyping with mixed reality technologies available online. I explored the following mixed reality technologies: Nearpod, ThingLink, Google Expeditions, EON Reality, Unity, Tinkercad and CoSpaces. Features of the envisioned prototype were isolated and tested with these technologies to evaluate their possibilities and limitations. In the end I chose online platform CoSpaces to develop the three-dimensional environment with.

Evaluation of the prototype

Two walkthroughs and semi-structured interviews. First, I asked the interviewees to think aloud during a walkthrough of the storyboard and the three-dimensional environment. Then, I held a semi-structured interview (see Appendix C for a list of the interview question). The first interviewee was a secondary school chemistry teacher and an educational designer. He had extensive experience with 3D modelling and with designing lesson materials about the topic of zeolites. The second interviewee was both a secondary school biology teacher and a secondary school chemistry teacher. He had some experience with 3D modelling and no experience with the topic of zeolites.

A short questionnaire with a group of secondary school chemistry teachers and chemistry teachers in training (n=17). The findings from the expert workshop and the resulting choices made in the developmental stage were evaluated with a second group of secondary school chemistry teachers and chemistry teachers in training. These were a different yet similar group of experts because they were attending a lecture in the same U-talent lecture series, yet about a different subject. The questionnaire can be found in appendix D.

Data analysis

The exploratory nature of this study led to a wealth of open-ended data. I engaged with the data through interactive reading, as described by Williams (2012). The data were subsequently divided into two groups: data from the developmental phase and data from the evaluative phase. From the developmental phase data categories and subcategories were extracted. The findings and design choices that were made in the developmental phase are described in light of these categories and subcategories. The categories and subcategories are:

1) Chemistry subject areas
    a) Secondary school level
    b) University level
2) Mixed reality technology
    a) Choosing a specific mixed reality technology
    b) Outsourcing the development

A priori themes were extracted from the developmental phase data to serve as input for the evaluative phase. These a priori themes brought focus to the questions asked in the semi-structured interviews. Additionally, they were used to code the walk-through and interview transcripts. The transcripts were read through and coded twice, once with a priori themes and once without, to ensure that remaining emergent themes were identified. A list of the a priori themes and emergent themes can be found in appendix E.

Results

1. Developmental phase

Chemistry subject areas

Secondary school level

Twenty-six experts (secondary school chemistry teachers and teachers in training) were observed during a workshop on the topic of virtual reality in chemistry education. In groups of three and four, participants were asked to design a lesson plan with virtual reality content relevant to their own teaching practice. Only two of the seven groups managed to come up with an outline for a lesson plan with virtual reality content. These two groups added virtual reality-content to their lesson plan with the explicit goal to increase student motivation and not to increase students' understanding of the subject. One of the experts stated that, in their opinion, secondary school students do not actually need three-dimensional images to understand the current chemistry curriculum. Another expert disagreed, stating that three-dimensional images are needed to understand stereoisomerism, which they found an admittedly small part of the secondary school chemistry curriculum.

Three other groups struggled with identifying the added value of virtual reality for their own teaching practice and as a result did not come up with a lesson plan. The two remaining groups stated that they were reluctant to try designing a lesson plan, because they feared it would give the researcher the wrong idea. One of the participants stated: "Virtual reality is just another thing you [educational researchers, red] are trying to ram down our throats. I am sick of it. We do not have enough time to teach our students everything in the curriculum and now you want us to add something completely irrelevant and unnecessary."

University level

Expert meetings with a professor of catalysis and a professor of inorganic chemistry focused on exploring the chemistry subject matter for which they could imagine using mixed reality.

The experts' need for mixed reality was found to be twofold. First, to validate their research and education; and second, to support their students. To validate their research and education, the professor of catalysis would like to use mixed reality technology to visualize concepts from green chemistry and sustainability research. Purification, synthesis, activation energy, active sites, carbon cracking and biomass catalysis with zeolites were identified as chemistry concepts likely to benefit from mixed reality.

According to the professor of inorganic chemistry, students often struggle to understand the limitations of different representations of atoms and molecules. Mixed reality was thought to be able to support these students, by allowing them to compare and zoom in on representations. Real-time mixed reality animations could then show the different representations' capabilities and limitations in being able to explain phenomena such as carbon cracking.

The experts coupled different types of mixed reality technology to specific chemistry concepts and learning activities. 360-Degree virtual reality movies were thought to be suitable for macro-level chemistry concepts such as synthesis and purification. The experts envisioned their students to be walking around in a chemical plant, looking at chemical reactions taking place on a large scale. They would then use virtual reality or augmented reality technology to zoom in on molecules and chemical reactions and zoom in even further to micro-level atom representations.

Both experts stated that mixed reality technology would need to be interactional to adequately support students. They envisioned their students being able to test (mis-)conceptions by: a) being able to zoom in and out at will; b) grabbing and manipulating molecules; and c) being able to control the passage of time in chemical reactions (i.e. starting or stopping a chemical reaction taking place).

The storyboard

Initially, I focused on university chemistry students as the target audience for the mixed reality tool, due to a perceived lack of need for three-dimensional imagery in the secondary school chemistry curriculum by the experts. However, early prototypes were dismissed by the experts for being overly simplified. The subject matter (carbon cracking with zeolites, a brief explanation about the topic can be found in Appendix A.) was found to be too complicated on a university level to be adequately developed by a researcher without expert level programming skills.

I subsequently explored the subject matter on the secondary school level. Secondary school *profielwerkstukken* (theses) and teaching materials were used to map concepts commonly used in relation to zeolites (see Appendix B). This concept map guided the development of the storyboard, of which you see an excerpt in Figure 2. Zeolites are not in the standard secondary school chemistry curriculum. The relevancy of the mixed reality tool was ensured by linking learning activities in the storyboard to examination requirements about sustainability and micro-macro-meso level reasoning. Figure 3 shows a flowchart linking macro- and meso level concepts to learning activities from the storyboard.

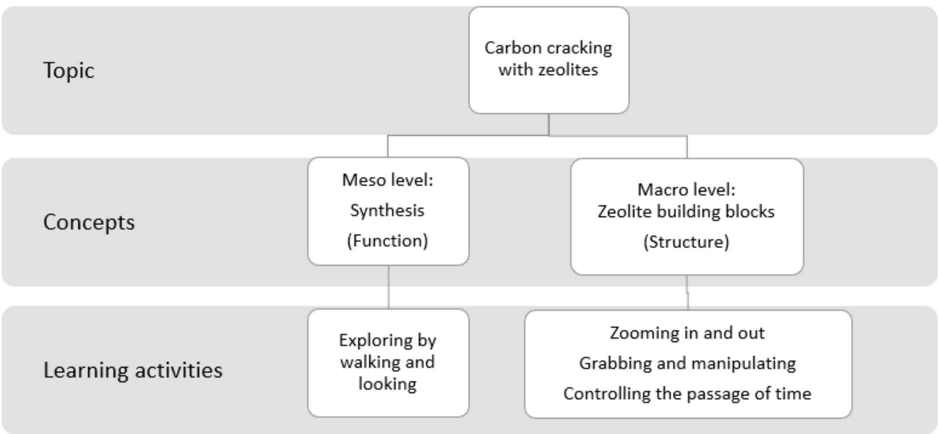

Figure 3. Flowchart linking concepts to learning activities.

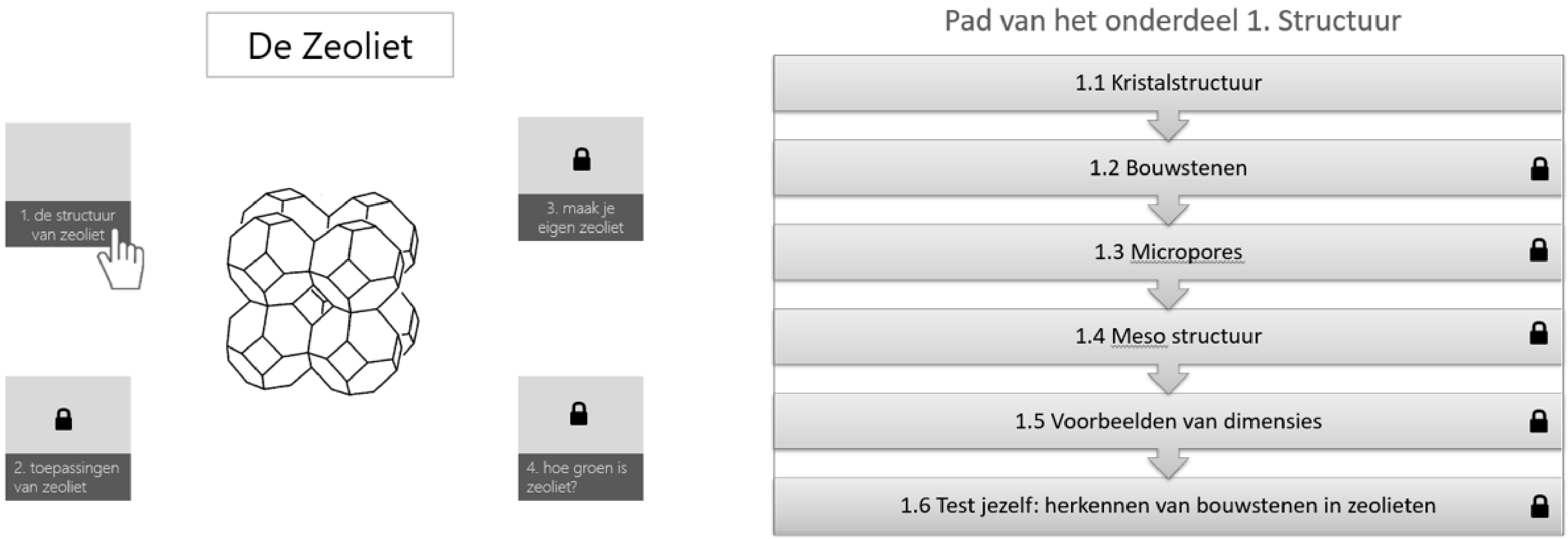

Figure 2. The first two slides of the developed storyboard for the mixed reality tool. Note: By selecting '*1. de structuur van zeoliet'* from the main menu in the left image, you enter the submenu in the right image. This submenu is a puzzle path with learning activities that you must complete before you can proceed to the next learning activity. You can only access the second option in the main menu ('2. toepassingen van zeoliet') when you have finished the first option. The first option focuses on understanding the structure of zeolite building blocks through activities in augmented reality and 3DoF virtual reality. The second options connects the structure to the function of zeolites with images in 360-degree virtual reality. The third options allows you to test your knowledge by constructing your own zeolite with 6DoF virtual reality. With the fourth option you consider different stakeholders and standpoints and decide how 'green' you think zeolites are.

Because of its inherently three-dimensional nature, I chose the structure of a zeolite building block to develop and study further. Only this part of the storyboard was developed with mixed reality in the next section of the study.

Mixed reality technology

Considerations in choosing a specific mixed reality technology

Expert meetings with a virtual reality researcher and an artificial intelligence researcher focused on the rationale behind choosing a specific type of mixed reality technology. The virtual reality researcher exclusively worked with ThingLink, a platform offering an online and desktop 360-degree editor. They chose this platform because it is easily accessible and has features that can be understood intuitively. These characteristics were found to be crucial for the type of research in question, lesson study, because the chemistry teachers involved did not have a programming background. The researcher considered using Google Expeditions but decided against it because adding and customizing a 360-degree environment is easier in ThingLink. Online platform TeachVR was considered as well but dismissed because it lies behind a paywall and is thus less accessible.

The artificial intelligence researcher often supervised virtual reality design studies and stated that 360-degree virtual reality platforms such as ThingLink are too limited for higher education purposes. 360-degree technology transports students to another place and time. However, it does not make the invisible visible. It was therefore the researcher’s opinion that 360-degree virtual reality is most suitable for vocational education, to connect theory with practice. For higher education purposes the expert prefers to work with mixed reality platforms that do make the invisible visible, such as TinkerCad and CoSpaces.

Tinkercad and CoSpaces are free for the most part and easy to master. Tinkercad can be used to design three-dimensional objects such as molecules, that can be uploaded into

CoSpaces. In CoSpaces, the programming language Code Blocks is then used to program the three-dimensional environment instead of more complex programming languages such as C#. The artificial intelligence researcher advised against using platforms with complex programming languages such as Unity and Blender. The learning curve would be too steep for non-programming educational designers.

Both CoSpaces and Tinkercad have starting 3D designers and children as their target audiences. Because of this, the artificial intelligence researcher stated that modelling complex molecular reactions in CoSpaces might be challenging. They did know of biochemistry researchers using CoSpaces to model protein folding with authentic research data, but a multidisciplinary team was needed to achieve this feat. The researcher hypothesized that randomly generating hydrocarbons with code blocks may be possible with Code Blocks. ‘Cracking’ colliding molecules into fragments might be simulated by turning part of the original molecule invisible.

Outsourcing prototype development

In this study, outsourcing the development of the prototype to professional developers was found to be tempting, because of the complexity of mixed reality technology. However, the artificial intelligence researcher did not recommend outsourcing. In their experience, it takes far too much time to bring an outsider up to speed on all the ins and outs of the project. As a result, the developed application is often not a true reflection of what the researcher had intended it to be.

With rapid prototyping it was found that developing simple prototypes yourself is in fact feasible and offers important benefits. Problems can be evaluated during the developmental process, decreasing the chances of ending up with a flawed product. Additionally, simple, self-developed prototypes may serve as comprehensible input for professional developers. This will result in less information being lost in translation between the designer and the developer.

The three-dimensional environment

Nearpod, ThingLink, Google Expeditions, EON Reality, Unity, Tinkercad and CoSpaces were evaluated with rapid prototyping. Based on the expert meetings and rapid prototyping, the following requirements were identified for the three-dimensional environment: a non-complex programming language, the ability to upload your own three-dimensional objects, the ability to make an animation with the uploaded object, and the ability to interact with the environment in preferably more than 3DoF. Table 1 shows how the platforms scored on each requirement. Online platform CoSpaces was selected as the most promising platform. Figure 4 shows an excerpt of the three-dimensional environment that was developed with CoSpaces.

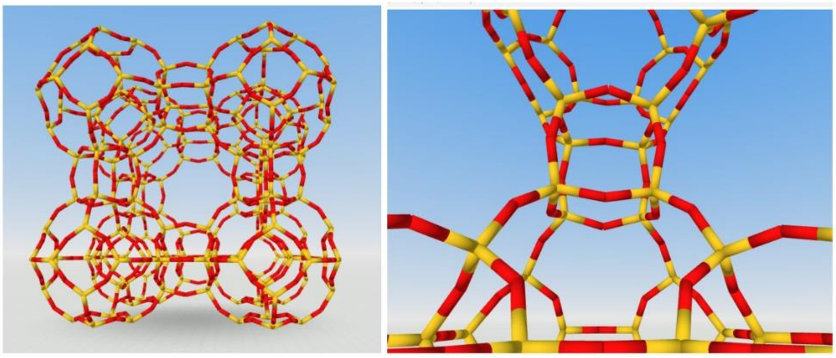

Figure 2. A look at the three-dimensional environment made with CoSpaces. Note: the left image is the outside view on a building block and the right image is what you see when you walk through the building block and look upwards.

Table 1. Characteristics of the online mixed reality platforms. Note: CoSpaces was found to be the most suitable platform to build a three-dimensional environment with.

Technology	Type	DoF	Object upload	Animation	Language	Target audience
Nearpod	360-degree VR	3	-	-	-	Teachers
ThingLink	360-degree VR	3	-	-	-	Teachers, students
Google Expedition	AR, 360-degree VR	3	No	-	-	Teachers, hobbyists
Eon Reality	AR, VR	6	No	Limited	-	Teachers, businesses
Unity	AR, VR	6	Yes	Yes	C# or Boo	Developers
Tinkercad	VR	3	No	Yes	CodeBlocks	Teachers, students
CoSpaces	***AR + VR***	***3***	***Yes***	***Yes***	***CodeBlocks***	***Teachers, students***

2. Evaluative phase

The prototype was evaluated with a questionnaire, walk-throughs of the prototype and semi-structured interviews with two experts: chemistry teacher and educational designer Coen Klein Douwel and biology- and chemistry teacher Mark Koren.

Curriculum concerns

Based on the findings from the expert workshops, the assumption was made that secondary school teachers would be hesitant to use a mixed reality tool about a topic not in the secondary school chemistry curriculum. Although zeolites are not currently in the curriculum, they are relevant in a sustainability context. In the final prototype, learning activities were therefore linked to sustainability examination requirements. The assumption was that this would increase teachers' willingness to use the prototype.

This assumption was checked with a questionnaire given to seventeen secondary school chemistry teachers and teachers in training. The results were unexpected. Sixteen of the seventeen secondary school chemistry teachers and teachers in training would use a virtual reality tool about the structure of zeolites, even without the sustainability context. Only one participant would not use the tool and not even when used in the sustainability context. This participant was the only participant attending both the expert workshop from the developmental phase and the lecture where the evaluative questionnaire was handed out. This suggests that the workshop participants may have been more critical about the added value of mixed reality, perhaps due to the lecture they had attended.

The questionnaire findings were echoed by the interviewees. For example, Klein-Douwel stated that he often diverts from the secondary school curriculum and finds a way to link a new topic to the existing curriculum. However, both interviewees stated that they know a lot of Dutch teachers who only do what the curriculum tells them to do. They predicted that linking zeolite learning activities to sustainability examination requirements would in fact increase the number of teachers who would use the prototype.

Supporting students' understanding of zeolites

The interviewees were cautiously optimistic about the prototype's potential to support students' understanding of zeolites. According to Koren, both his students and he himself find it difficult to mentally mirror and rotate the structure of complex molecules. So difficult in fact, that he often resorts to teaching his students tricks: *'Are there four different groups surrounding the C atom? If so, that makes it an asymmetrical C-atom and you need to multiply the number of mirror-isomers times two to answer the question"*. According to Koren, walking around and through the building blocks of a zeolite in virtual reality would aid his students in understanding and constructing a three-dimensional mental image. This in turn would make it easier to transform and reason with the building blocks.

Klein Douwel appreciated the ability to walk through a zeolite in virtual reality. He himself once considered having his students build physical three-dimensional models of zeolites with a 3D-printer. However, students would not be able to enter the cavity in a physical model, which would limit their understanding of the function of the cavity. Klein Douwel considered walking through the three-dimensional model in virtual reality a viable alternative.

Being able to reason with macro-level building blocks is necessary when students need to consider the implications of a structural characteristic on a meso-level. Koren stated that micro-macro-meso level reasoning is a skill that students often struggle with. They have trouble finding the right words to describe the function of a molecule on a meso-level. Klein Douwel echoed this sentiment, stating that students often have trouble translating an image to language and then to a reaction mechanism. According to Koren, experiencing the words and their meaning in virtual reality would make it easier to correctly couple the words to meso-level phenomena, such as the use of zeolites in water purification or cat litter.

Limitations of the prototype

Although Koren was optimistic about the added value of the prototype for the chemistry classroom, he stated that he would probably not use it. He would never want to rely on the school's spotty Wi-Fi connection and he in fact uses as little technology as possible in his classroom. Downloading the prototype to a device in advance of the lesson could be a solution, however, that is not an option with the current prototype. Additionally, Koren feared that the prototype would not be compatible with all of his students' personal devices. Cheaper mobile phones often do not have the gyroscope and/or accelerometer necessary to execute virtual reality.

Both Koren and Klein Douwel stated that they certain missed features that would make the prototype more interactive. These features would be the ability to grab and manipulate objects and to influence the passage of time. According to Koren, adding this interactivity would have two possible learning effects: it would increase students' motivation and their understanding of the subject. Klein Douwel agreed that the ability to test (mis)conceptions would support students' understanding of zeolites. He said: "*What you would really want is to grab the molecule, take it to an active site and see what happens: some things are impossible, and others do create a bond*."

A simple stick model was used as the representation for the zeolite building block in the prototype (see Figure 5a). Klein Douwel spotted an important problem with this representation. It creates the misconception that a zeolite has more entry points than it actually has. "*Right now, you can see holes in the molecule and so it seems like you could go in there, but that is not true at all. (...) You need van der Waals surfaces to really show shape* *selectivity."* Figure 5b shows the more accurate Van der Waals representation of the zeolite building block. This representation is less striking and easy to understand than the simple stick model. A compromise might be the representation in Figure 5c, showing both the stick model and some Van der Waals surfaces. However, walking through and looking through an unobstructed building block is only possible with the simple stick model.

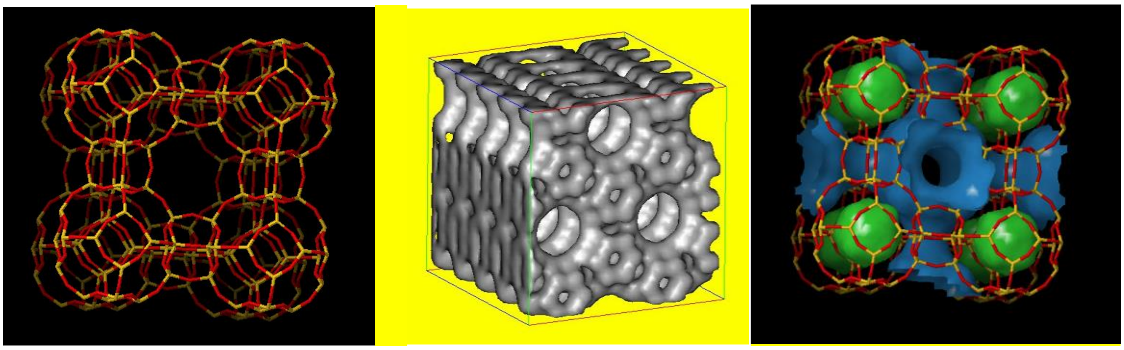

Figure 3. Representations of a zeolite building block. Note: the image on the left (a) is a simple stick model. The image in the middle (b) shows van der Waals surfaces. The image on the right (c) is a combination of the previous two images. Adapted from the online Database of Zeolite Structures.

Expanding the learning activities

Klein Douwel and Koren were asked to comment on the learning activities currently in the prototype. Both would prefer there be more math problem activities. According to Klein Douwel, math is one of the languages of chemistry that students must speak and should therefore be integrated in all subjects. Koren stated that 80% of the final chemistry exam ('*eindexamen'* in Dutch) assignments contain calculations. Because Koren wants his students to do well on the final exam, adding calculation activities to the prototype would increase the chance that he would use it in his classroom.

Koren suggested asking students to determine the ratio of silicon and aluminum in the building blocks of zeolites. Students would be familiar with these types of calculations from determining the ratio of ions in a salt. Koren felt that calculations would not only help the students practice for the final exam, but also support their understanding of the structure of zeolite building blocks and their function.

The target audience of the prototype was 11^{th} and 12^{th} grade secondary school chemistry students. Koren could envision using the prototype as early as the 9^{th} grade and continue using the prototype in every grade every year. He would use the prototype as a form of discovery-based learning. In the 9^{th} grade he would show his students the three-dimensional environment without giving them an explanation. "*What kind of characteristics do you see and what could that mean for the function of this molecule? (...) I'm curious to see if they can recognize things they have already learned about*." In later years he would add calculation activities and the more formal linking of concepts with the three-dimensional images.

Discussion

The aim of this study was to explore considerations in the design process of a mixed reality tool that supports chemistry students' understanding of zeolites. The findings are by no means exhaustive and must not be interpreted as such. They can however serve as an example or starting point for other educational designers and chemistry teachers. Additionally, the findings will most likely be used as input for the (outsourced) development of a mixed reality tool by the Freudenthal Institute.

Motivation for the design

The most important consideration in the design process of a mixed reality tool was found to be the motivation for the design. The motivation heavily influences the choices and sequence of choices that must made in a design process. Few of the parties and platforms investigated in this study were transparent about their motivation. Educational mixed reality design was found to be a complex tangle of science, business, and education interests (as may be the case for most innovative educational technologies). Still, five possible motivations were identified.

First, the tool may be developed in response to a student problem encountered by a teacher or teachers. In that case the subject area or usage scenario serves as the starting point of the design process. Second, the tool may be designed with a specific learning outcome in mind from the cognitive, affective, or conative domain. A decision must be made to support either students' understanding, motivation, or the development of a specific skill. Third, the tool may be developed to validate research and promote a research group or research institution. This motivation is most relevant for university level mixed reality tools. Fourth, only a single mixed reality technology is explored and serves as a starting point in the design. This may be because of required technology features or existing institutional contracts. Fifth, as was the case in this study, subject areas and usage scenarios are explored in an effort to identify where and how mixed reality technology can be most useful.

These five motivations do not exclude one another. In fact, any remaining motivations represent the choices that must be made in a later stage of the design process. In this study, exploring where and how mixed reality technology can be most useful in chemistry education was chosen as a starting point. The cognitive domain - supporting students' understanding - was chosen to bring focus to the research question. Chemistry subject areas in secondary school and university were subsequently explored, with secondary school being the chosen education level. Only then was the chemistry subject area 'zeolites' selected and, finally, the mixed reality platform CoSpaces.

Subject areas, learning processes and learning activities

In secondary school, only one subject area currently in the curriculum could be identified to benefit from mixed reality: stereoisomerism. It was easier to identify subject areas in the university curriculum because it more often required students to make a mental three-dimensional image. However, mixed reality images for university students needed to be a great deal more accurate and authentic than images for secondary school students. The technology needed to create these accurate and authentic images is more complex. I myself, being an educational researcher without programming experience, found it impossible create accurate and authentic images suitable for university education.

Stereoisomerism is only a small part of the secondary school chemistry curriculum. That is why, during the expert workshop, secondary school teachers struggled to find the added value of mixed reality for their lesson plans. It was found to be more fruitful to identify chemistry learning processes and learning activities that may be supported with mixed reality. Micro-macro-meso level reasoning is one of those learning processes. To facilitate and stimulate micro-macro-meso level reasoning, the overarching subject ‘carbon cracking with zeolites’ was chosen for this study. The storyboard connects meso level concepts such as catalysis to macrolevel building blocks of zeolites and to microlevel atoms and electromagnetic forces. Even though zeolites are currently not in the curriculum, reasoning about the function of a zeolite in relation to its structure was found to make the tool more relevant. Educational designers and teachers who struggle to find the added value of mixed reality technology are therefore recommended to explore learning processes and activities in addition to subject area(s).

Outsourcing and early prototyping

Chemistry students gain understanding in mixed reality by zooming in and out, grabbing and manipulating building blocks, and starting and stopping chemical reactions. 360-Degree virtual reality is a form of 3DoF stationary virtual reality and cannot facilitate these interactions. To achieve interactivity, one needs the ability to upload three-dimensional objects, and to animate these objects in preferably more than three DoF. Because this requires a more complex programming language, many educational designers and researchers choose to outsource the development.

However, this study showed that it is beneficial to develop early prototypes yourself, at least when the target audience is secondary school. While the developed three-dimensional environment certainly has its shortcomings, valuable insights came from its development and evaluation. The same cannot be said about university level mixed reality tools. These tools were found to be too complex to prototype on platforms such as CoSpaces. A possible solution may be to jointly develop early prototypes with a multidisciplinary team consisting of an educational researcher, a mixed reality programmer, and a chemistry researcher.

Further research

Several areas of research were identified that may be further explored. First, representations of atoms and molecules can either help or hinder a student's understanding of mixed reality. Many consider van der Waals surfaces to be more accurate and insightful than simple stick models. It is however unclear if this holds true for mixed reality. Walking through a molecule with van der Waals surfaces could be confusing and thus hinder a student's understanding of the structure. Although they were found to cause misconceptions, simple stick models seem easier to understand in mixed reality. Additionally, some representations may be more suitable for a specific type of mixed reality technology. Van der Waals surfaces, for instance, could only be problematic when you walk through a molecule in virtual reality and not when you look at the molecule with augmented reality.

A second area of interest is the factors that influence the usability of a mixed reality tool. One of the interviewees feared that the tool would be too dependent on a Wi-Fi connection and not compatible with students' personal devices. This may mean that a tool will not be used, even when teachers are positive about the content. Possible solution directions are downloadable content and standalone devices. Adding (ratio)calculations may increase the uptake of a tool as well, since a large part of the final chemistry examination consists of calculations. Practical concerns like these should be addressed before developing the final prototype.

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Appendix

Appendix A: Carbon cracking with zeolites

Zeolite chemistry is often taught during undergraduate catalysis courses. In a commonly used textbook for students, Hanefeld and Lefferts[1] state the following about zeolites:

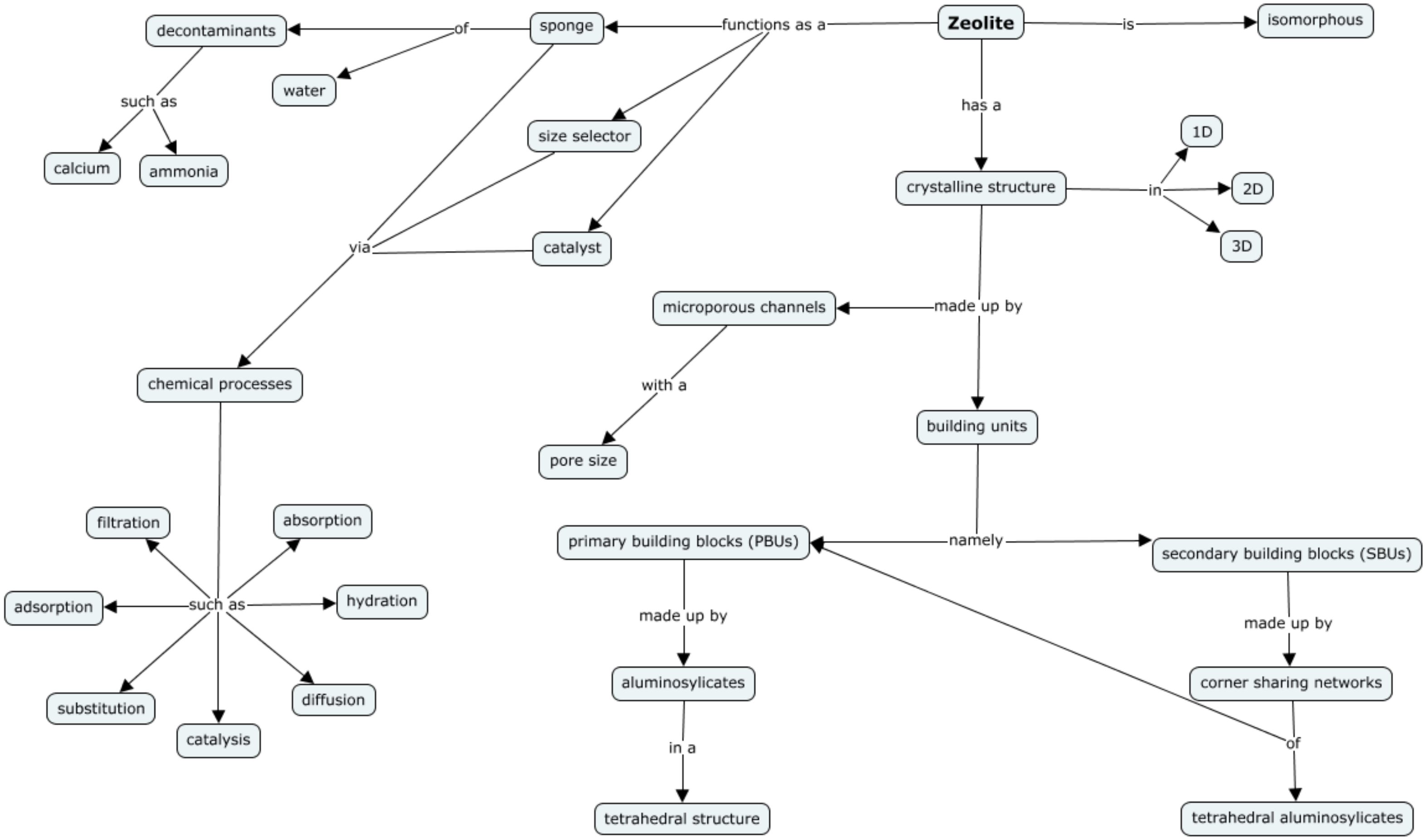
> Zeolites, for instance, are used in cracking of heavy oil feedstock. Zeolites are crystalline aluminosilicates that assemble into well-defined three-dimensional structures composed of microporous channels that interconnect cavities with dimensions approaching those of molecules, that is, sizes around 2-20 Å. (…) Besides their use as a water softener, zeolites are used as solid acid catalysts in a large number of commercial processes such as catalytic cracking of heavy oil to gasoline, hydrocracking gas oil to diesel and kerosene (…). (p.63-64)

And:

> The primary building block of the zeolite structure is the TO_4 unit (…), a tetrahedron consisting of a central metal cation (usually Si^{4+}) and four (much larger) oxygen anions. The tetrahedra can be connected in different ways to form a three-dimensional structure by sharing corners, edges, or planes. By combining primary building blocks, secondary building blocks can be constructed, such as flat four- or six-rings. These can then be further assembled in larger composite building units, such as the sodalite cage (…) Arrangement of these larger units into the crystalline zeolite structure determines the porosity of the zeolite, comprising cages, cavities, and/or channels. (p.327)

[1] Hanefeld, U. & Lefferts, L. (2018). Catalysis: An Integrated Textbook for Students. Germany, Weinheim: Wiley-VCH.

Appendix B: Concept map



Appendix C: Semi-structured interviews

Table B1 Interview questions Koren

Vragen	Prompts
Introductie (ijsbrekers)	
Hoe zou je jezelf beschrijven als docent?	Wat onderscheidt jou van andere docenten? Wat zijn jouw kenmerken?
Welke klassen geef je les?	
Hoe lang al?	
Heb je al eens iets gedaan met VR?	Met de klas? Zelf? Nascholingsdag?
Interview	
Gebruik je wel eens innovatieve technologie in de klas?	Waarom gebruik je die? / Waarom niet? Wat zijn je ervaringen?
Op wat voor manier zijn jullie met duurzaamheid bezig in de klas?	Wat staat er in de boeken? Is het verschillend per leerjaar?
Welke molecuulrepresentaties gebruik jij in de klas?	Ball and stick? Orbitaal theorie? Newton? Van der Waals?
Zijn er in de scheikunde onderwerpen waarbij leerlingen zich de 3D structuur van moleculen voor moeten kunnen stellen?	Mentaal model? Spiegelen? Isomeren?
Merk je weleens dat leerlingen het moeilijk hebben met schakelen tussen 2D en 3D?	Wat vinden ze moeilijk? Heeft inzicht er iets mee te maken?
Op wat voor manier zou jij VR willen gebruiken in de klas?	Kun je je daar iets bij voorstellen? Voor welke onderwerpen bijvoorbeeld?
Walk through – Storyboard	
Is er een onderdeel dat anders zou moeten?	Mis je iets? Een onderdeel waarvan je denkt ‘dat moet je niet doen’? Wat voegt VR hier aan toe?
Walk through – 3D Omgeving	
Kun je je voorstellen dat leerlingen er iets aan hebben om door het molecuul heen te lopen?	Wat leren zij er van?
Mist er iets?	Interactiviteit? Is lopen genoeg voor begripsvorming?
Wat denk je dat leerlingen ervan vinden?	Motiveert het? Leidt het af?
Interview	
Is er nog iets dat je toe zou willen voegen aan de app?	Wat zou je anders doen?
Is er nog iets wat je kwijt wil of wil vragen?	

Table B2 Interview questions Klein Douwel

Vragen	**Prompts**
Introductie (ijsbrekers)	
Waarom hebben jullie (U-talent, red) voor het onderwerp zeolieten gekozen?	
Kun je me iets vertellen over je ervaring met de module zeolieten?	
Interview	
Zijn er leerlingen die moeite hebben met ruimtelijk inzicht?	Wat vinden ze dan zo moeilijk?
Wanneer geeft een 3D model extra inzicht?	Verschil met computermodel en fysiek model?
	Verschil met VR model?
Wat vinden leerlingen het moeilijkst aan de module zeolieten?	
Merk je weleens dat leerlingen het moeilijk hebben met schakelen tussen 2D en 3D?	Wat vinden ze moeilijk?
	Heeft inzicht er iets mee te maken?
Op wat voor manier zou jij VR willen gebruiken in de klas?	Kun je je daar iets bij voorstellen?
	Voor welke onderwerpen bijvoorbeeld?
Walk through – Storyboard	
Is er een onderdeel dat anders zou moeten?	Mis je iets?
	Een onderdeel waarvan je denkt 'dat moet je niet doen'?
	Wat voegt VR hier aan toe?
Walk through – 3D Omgeving	
Kun je je voorstellen dat leerlingen er iets aan hebben om door het molecuul heen te lopen?	Wat leren zij er van?
Mist er iets?	Interactiviteit?
	Is lopen genoeg voor begripsvorming?
Wat denk je dat leerlingen ervan vinden?	Motiveert het?
	Leidt het af?
Interview	
Is er nog iets dat je toe zou willen voegen aan de app?	Wat zou je anders doen?
Is er nog iets wat je kwijt wil of wil vragen?	

Appendix D: Questionnaire

The following questionnaire was handed out so seventeen secondary school chemistry teachers and chemistry teachers in training:

Wij zijn bezig met het maken van een Virtual Reality-app. Met de app kunnen leerlingen rondlopen in de driedimensionale structuur van een zeoliet (een poreus macromolecuul). De leerlingen kunnen daarbij zelf ondervinden hoe de structuur van de zeoliet bepalend is voor, onder andere, de katalytische functie.

1. Zou jij de app in de klas willen gebruiken? (vink één vakje aan)

O Ja → *Je bent klaar*

O Nee → *Ga naar vraag 2*

2. Zou jij de app wel willen gebruiken als het in de context van duurzaamheid plaatsvindt? (vink één vakje aan)

O Ja → *Je bent klaar*

O Nee → *Ga naar vraag 3*

3. Waarom niet?

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Bedankt voor het invullen van de vragenlijst!

Als je vragen hebt over de app of mee wilt doen aan het testen van de app kun je mailen naar **@students.uu.nl of naar **@uu.nl.

Appendix E: Labeling system

Table D Labeling system used in the coding of the data.

Theme	Description
	A priori
Curriculum	An expression about the place of a topic in the secondary school chemistry curriculum
3D mental images	An expression about the models and images students must create in their own minds after seeing a picture or hearing a description of a concept
Stereoisomerism	An expression about the topic stereoisomerism in relation to either 3D mental images or MR technology
Added value of MR	An expression about the value of MR relative to other technologies or pedagogies
Visualizing concepts	An expression about the act of translating the description of a concept to a movement, image, or animation
Carbon cracking with zeolites	An expression about the role of zeolites in the process of carbon cracking
Catalysis	An expression about the chemical process of catalysis or about a concept relating to catalysis, such as activation energy or purification
Representations A	An expression about the various representations of atoms, such as the Dalton, Thomson, or Rutherford model
Micro-meso-macro	An expression about the coupling of micro-level concepts to meso- and macro-level phenomena and vice versa
Zooming in and out	An expression about the act of zooming in and out on an image or animation in order to gain a better understanding of the subject
Grabbing and manipulating	An expression about the act of grabbing and manipulating (part of) an image or animation in order to gain a better understanding of the subject
Controlling the passage of time	An expression about the act of starting or stopping an action or reaction in order to gain a better understanding of the subject
	Emergent
Practical concerns	An expression about the feasibility or usability of the prototype
Sustainability	An expression about the topic of sustainability in chemistry education, either in relation to the curriculum or in relation to the prototype
Modeling	An expression about the topic of modeling in chemistry education, either in relation to the curriculum or in relation to the prototype

Spatial ability	An expression about the ability to understand, translate and transform a three-dimensional image of a molecule
Envisioning the use of MR	An expression about needing or wanting to use MR technology to better visualize or understand a concept or topic
Calculations	An expression about the use of calculations in chemistry education, either in relation to the curriculum or in relation to the prototype
Interactivity	An expression about the ability of the prototype to respond to student or teacher input
Extra functionalities	An expression about adding a function or property to the prototype.
Representations B	An expression about the various representations of atoms in molecule models, such as the ball-and-stick model or Van der Waals surfaces.