Characterising Structure-Property Reasoning within a Chemical Design Challenge: 'Green Bubble Soap'

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ABSTRACT

Where design seems to merge easily with physics or technology education, it does not seem to take place in secondary chemistry education. Design is one of the crosscutting concepts between the different STEM subjects, (Science, Technology, Engineering, Mathematics) and is therefore included in curricula and standards in many countries. Function-Behaviour-Structure (FBS) reasoning is an important design skill. In a chemical context it shows similarities with structure-property reasoning (SPR). This SPR is a common practice for chemical engineers but difficult to learn for secondary students. Given the similarities, chemical design activities might be a way to enhance students' SPR. Moreover, SPR might be a useful tool in the FBS framework when evaluating behaviour derived from a micro level structure. We describe an explorative study in which the design of bubble soap is used as a context to promote students' SPR. Data was collected in the form of audio recordings of student conversations within the design team and their design drawings on worksheets. Qualitative analysis, using the perspective for SPR as a framework, revealed that identified SPR was expressed in three ways: as a link between structural features and substances, as a link between the term 'molecule' and property and as a link between molecular structures and properties of a substance. Furthermore, analysis showed that SPR was only found during evaluation, discussion and ideation stages of the design process. The results indicate that this chemical design project can be used to stimulate students' SPR and that SPR can be related to processes of the FBS framework.

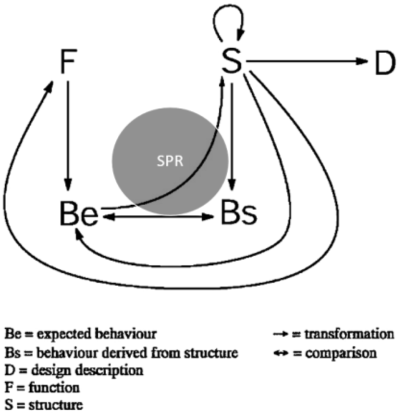
Key Words: Structure-property reasoning, Function-behaviour-structure thinking, Design-based learning, Chemical Engineering.

1. INTRODUCTION

In the last decades, design-based teaching approaches have gained significant attention from researchers. Design has been part of STEM curricula in many countries (NGSS, 2013; CvTE, 2022). Design activities serve as a vehicle for teaching and learning science concepts within a problem-solving context (Fortus et al., 2004; Apedoe et al., 2021). In some cases, these activities can be more effective than a scripted inquiry (Mehalik et al., 2008; Guzey & Jung, 2021). Furthermore, design activities can lead to improvement of students' scientific reasoning (Chusinkunawut et al., 2021). The design process consists of different stages such as 'identification and research of the problem', 'ideation', 'constructing and testing the prototype', 'discussing results' and 'evaluating the test outcomes'. Students' reasoning varies throughout these different stages (Aranda et al., 2020). STEM education can also contribute to the learning of design skills in different contexts. Therefore, integrating design in STEM education benefits both ways (Li et al., 2019). The technoscientific nature of chemistry, one of the science disciplines in STEM education, is manifested in the core practices of chemical engineers: design and synthesis of molecules and materials, exploring novel synthesis routes, analysis and optimisation of processes, all for people to extend their abilities and to satisfy their needs and wants (Talanquer, 2013). A biochemical engineering example is the synthesis of liposomes for controlled drug delivery (Nguyen et al., 2014). Design activities therefore can serve as an authentic practice to involve secondary students in the way chemical engineers think and do. But where design seems to merge easily with physics and technology education it does not seem to take place much in upper secondary chemistry education (Roehrig et al., 2012; Stammes et al., 2020).

In technology and engineering design, Function-behaviour-structure (FBS) thinking is an important concept. The FBS framework (figure 1) describes a way of relating structural components of a design to their function and the mechanisms that enable them to perform their functions (Gero & Kannengieser, 2004). The FBS framework describes processes that connect the function variables (what is it for?), via the expected- and structure-derived behaviour variables (what it does), with the structure variables (what it is) to eventually end up with a design description. Different from engineering design, in a chemical design activity the processes of evaluation and synthesis require reasoning about the structures on a non-observable molecular level, emergent observable properties at macro level and then linking these with expected- and structure-derived behaviour. Furthermore, chemical engineers hypothesize what structures at micro level can account for the desired properties of a material at a macroscopic level (Sevian & Talanquer, 2014). By providing explanations or predictions in this manner, they apply what is called 'structure-property reasoning' (SPR). SPR is a chemistry-authentic practice and it is embedded in many chemistry curricula (NGSS, 2013; CvTE, 2022). Chemical engineers use this way of thinking seemingly easy, but structure-property reasoning is difficult to master for novice learners (Chi et al., 2012; Johnstone, 1997).

Figure 1.
The FBS framework adapted from Gero & Kannengiesser (2004). The grey sphere indicates where SPR is situated within the FBS framework.



A good understanding of structure-property relations can help students to better understand chemistry concepts (Talanquer, 2018) and make better design decisions. The similarity of structure-behaviour-function thinking in design and SPR in chemistry might provide a possibility to integrate design into chemistry classrooms and stimulate students' SPR. Moreover, SPR may provide a useful tool in the FBS framework when evaluating design behaviour in relation to molecular structures. A way to introduce SPR is by using perspectives as a lens to approach an observable phenomenon. In general, a perspective guides the students in asking questions and assessing their answers by *"...lighting up a certain aspect of the real world and directs the research on those aspects."* (Janssen et al., 2020 p.255). The perspective for SPR provides specific questions to guide students' reasoning from macro level to micro level (Den Otter et al., 2021). An adapted version of this perspective (figure 2) can serve as a framework to characterize students' expressions.

Figure 2.
Perspective for Structure-Property reasoning.

Students' way of reasoning cannot be investigated directly. We can only look at representations of their thoughts. In the situated FBS framework drawings, for instance, are referred to as the 'externalised expected structure' (Gero & Kannengieser, 2004). The students' drawings of molecular structures and their speech, represent the way the students think about matter on a macro or micro level and can provide information to assess students ways of chemical thinking (Taber, 2013, Stammes et al., 2023). However, specific research on secondary students' SPR during engagement in chemical design activities is scarce.

For our studies purpose, a project around the design of bubble soap was used, as we will describe in section 2.1. Bubbles find a technological application in drug delivery, food technology and waste water treatment (e.g. Kaushik & Chel, 2014). In this paper, we describe a small scale explorative study we performed to gain more insight in students' SPR while engaged in this specific design challenge, called 'Green bubble soap'. We aim to answer the following questions:

- In what way can students' identified structure-property reasoning be characterized during engagement in the chemical design activity 'Green bubble soap' in upper secondary chemistry education?
- What relationship can be identified between students' structure-property reasoning and the different stages of the chemical design project 'Green bubble soap'?

2. METHODOLOGY

2.1. Context

The project 'green bubble soap' was used to teach in a 10^{th} grade secondary chemistry class two obligatory parts of the syllabus: solubility of compounds and design skills. This was done during three subsequent, regular time-tabled lessons of 45 minutes in May 2023:

(i) Lesson 1: An introduction on design in general, an introduction of the project, the demands of the desired product and generating ideas on volume-ratios of water-soap mixtures.

(ii) Lesson 2: A small experiment to guide students' thinking about the behaviour of soap molecules in water. Building and testing of the artefact, discussing the results with the teacher, redesign and generating ideas.

(iii) Lesson 3: Building and testing the final prototype and wrap-up of the project: What is the recipe for the best bubble soap, the design description. How to become the Bubble Boss?

The goal of the design project was to identify the recipe for the perfect bubble soap with sustainable / natural ingredients. The definition of 'perfect' was first established and came down to "long lasting bubbles". Students had to specify the required properties of the bubble soap, the expected behaviour, and subsequently propose ideas for an additional ingredient besides water and soap to better meet the expected behaviour. While generating ideas or evaluating test results, students were encouraged to explain their decisions with the use of SPR.

2.2. Participants

All of the participants were connected to a secondary school in an urban area in the west of the Netherlands. Convenience sampling was applied for our study in which we focus on two student teams. Each team consisted of 2 male students aged between 15 and 17 years old ($n = 4$). The teacher guiding the design challenge works as chemistry teacher in that school, and is the first author of this article. He holds a master's degree in chemistry, is qualified for teaching upper secondary chemistry classes and has 14 years of teaching experience. The two student teams were chosen for being 'easy talkers'. Since we want to capture representations of thought, we wanted to gather as much talk within a group as possible within a lesson. The two teams were asked to cooperate and were fully informed about the purpose of our study, the way the data was collected and stored, and they subsequently gave their consent.

2.3. Data collection

We collected the data during the second lesson because this lesson was the most student-centred lesson of the three. Therefore, this lesson would generate the most student talk during the different stages. We asked students to express their thoughts out loud. The talks within each team and with the teacher was audio recorded and transcribed verbatim. In addition, we used a set of worksheets per team (Stammes et al., 2023) for students to draw and sketch their micro-level structures on. Furthermore, the worksheets had pre-structured questions for students to answer, to guide the design process. The students' worksheets with drawings and written reasoning were digitalized as pdf-file.

2.4. Data analysis

First the transcripts were divided in sections and marked according to the different stages of the design process, using ATLAS.ti. After that, a deductive coding approach was employed where the transcripts were recoded using questions of the perspective for SPR (figure 2) as an analytical lens.

Table 1.
Examples of students' expressions underlying the applied codes.

Codes	Example of students' expression
Macro – substance	"*we take water and soap*"
Macro – organisation	"*bubble" / "we got layers" / "3 millilitre and 7 millilitre ratio*"
Macro - property of substance	"*sugar is hydrophilic" / "it dissolves well*"
Micro – type of particle	"*The water molecules…" / H's and O's*"
Micro – interaction	"*They have strong bonds*"
Micro – organisation	"*We have 2 water molecules on 1 soap molecule*"
SPR	"*A lot of bonds to be hydrophilic, a lot of O-H bonds, or N-H*"

Students worksheets and drawings were coded using the same approach. First by stage of the design process and then recoded using the perspective for SPR. The selected quotes and applied codes were discussed between the first and second author until a consensus was reached about whether a quote was to be selected or not and whether it expressed thoughts on a micro level, macro level or SPR. If no consensus was reached, the quotes were left out of the analysis. The code co-occurrence tool in ATLAS.ti then revealed in what stages of the design process SPR codes occurred.

Subsequently all quotes with the applied code 'SPR' were grouped and axial coded to uncover themes and characterize the expressed reasoning.

3. RESULTS AND DISCUSSION

3.1. Characterizing the identified SPR

Our first research question was: In what way can students' identified structure-property reasoning be characterized during engagement in the chemical design activity 'Green bubble soap' in upper secondary chemistry education?

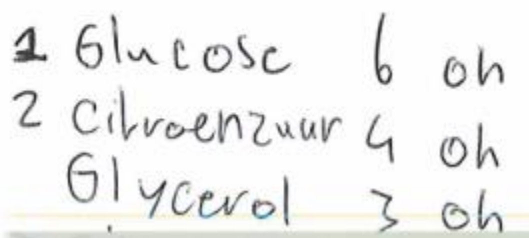
Analysis of the fragments with the applied code 'SPR' revealed that it was expressed by students in one of three following ways:

3.1.1. A link between substances and their structural features.
The first category of students' SPR expressions contained a link between a substance and the structural features or characteristic moieties of the molecules. The following quote provides an example.

> Student 1: You want one with O-H bonds, right? Well, then there is glycerol, citric acid.

When looking at the FBS framework, this type of thinking emerges in the proces of reformulation of the structure when new structure variables are introduced. They also annotated it on their worksheets with ideas:

Figure 3:
Annotation of ideas for substances on the worksheet, ranked by the number of OH-groups in the molecule. [citroenzuur] means citric acid.



3.1.2. A link between the term '...molecule' and properties.

The second category we identified contained verbal or written expressions in which macro level properties were attached to specific molecules.

> "A soap molecule can dissolve with one or two water molecules"

In this example, the property 'dissolving' is linked to the micro-level term 'soap molecule'. This expression was used by students to explain an observed test result, which in the FBS framework aligns with the process of evaluating expected- versus structure-derived behaviour.

Or as students described on their worksheet :

> The hydrophobic part of the soap molecule pushes the pepper to the side.

In this excerpt students describe an observed behaviour: the pepper floating on a water surface in a bowl being pushed to the sides when a drop of bubble soap is added. They link the property hydrophobicity to a part of the soap molecule. Moreover it explains for them a structure-derived behaviour.

3.1.3. A direct link between structural features and the properties.

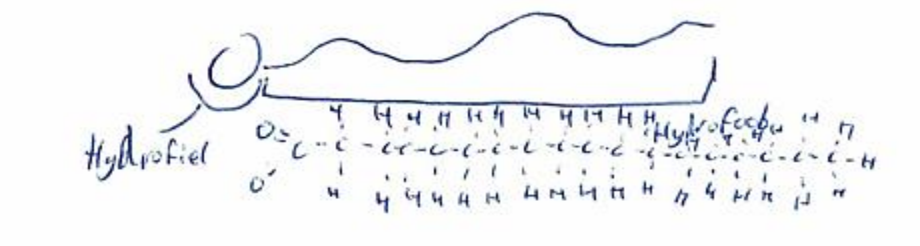
When evaluating the test results of their prototype, and subsequent ideation, group 1 expressed a direct link between structural features and properties in the following way:

> Student 2: A hydrofobic compound, a hydrophilic compound I mean.
>
> Teacher: A hydrophilic compound, So you're looking for a molecule that...What requirements does such a molecule have to meet, when it is hydrophilic?
>
> Student 2: A lot of bonds to be hydrophilic, a lot of O-H bonds, or N-H"

In the example above we see that the identified SPR was guided by the teacher. The reasoning itself began at macro level property, 'hydrophilic', via statement at micro level interaction, 'bonds', to statements at micro level about structural features of the desired molecules. In relation to the FBS framework this describes the process of synthesis: going from expected behaviour to structural features.

We also saw this structure-property link, hydrophobicity and a branch of C-atoms in the structure, in an annotated drawing (figure 4).

Figure 4. Annotated drawing of a soap molecule. [hydrofiel] means hydrophilic and [hydrofoob] means hydrophobic.



3.2. SPR per stage of the design project

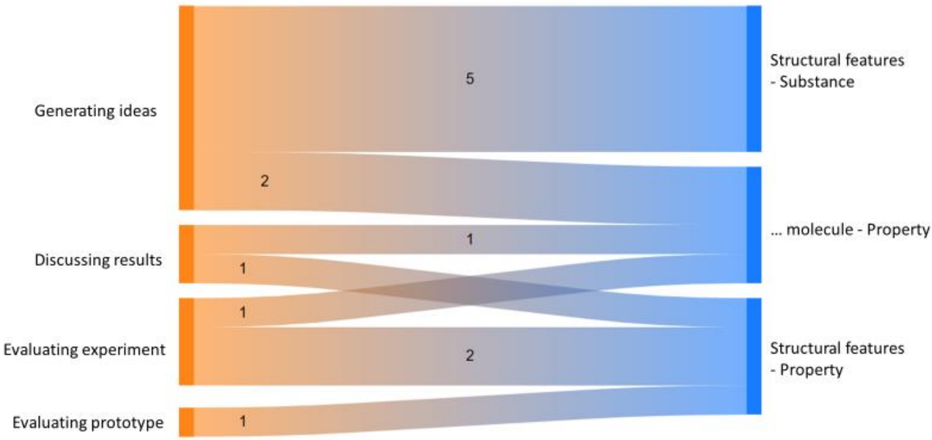
The second research question guiding our analysis was: What relationships can be identified between students' SPR and the different stages of the chemical design project 'Green bubble soap'? We identified (grey in table 2) many expressions about the micro and the macro level, but only in four stages of the design project SPR was identified. When performing the experiment, building the prototype, and testing the prototype students expressed no direct SPR.

Table 2.
Identified micro level, macro level and SPR expressions per stage of the design process.

	Macro - organisation	Macro - property	Macro - substance	Micro – Type of particle	Micro - interaction	Micro - organisation	SPR
Evaluating prototype							
Generating ideas							
Evaluating experiment							
Performing experiment							
Prototype building							
Prototype testing							
Discussing results							

3.2.1. Stages of the design project in which SPR was identified
As described in section 3.1, identified students' SPR could be divided into three categories: a link between structural features and substances, a link between the term 'molecule' and properties and a link between structural features and properties. The structural feature – substance link was only found in the stage of generating ideas (figure 5).

Figure 5.
Sankey diagram of stages of the design activity in which SPR links were identified.



When generating new ideas, students in group 1 used structural features to select the ingredient that they thought would improve their design. They then compared the molecular structures of the substances given, to select the molecule with the highest amount of hydroxyl groups as being the best candidate to meet the expected behaviour.

> Student 1: Structure formula. You want one with O-H bonds, right? Well, then there is glycerol, citric acid.
>
> Student 2: No, regular salt is not going to work.
>
> Student 1: glucose has H's. [looking up structures on their smartphones]
>
> Student 2: Glucose, WOW! That's the one, that's the one! All right.
>
> Student 1: no, no, we keep that one in mind. How many OH?

The students remained in the stage of generating ideas and weighing all compounds to make sure one of the candidates stands out as being the best one.

In contrast, when we looked at group 2, no SPR was observed in the stage of ideation. In this stage they stuck to the macro level descriptions of substances and rushed into the stage of building and testing their new prototype.

> Student 3: Shall we just begin with sugar? I always used to do it with sugar in it.

Student 4: You always used sugar?

Teacher: …

Student 4: Yes, let’s just do that.”

In the stages of evaluating the prototype, evaluating the experiment, and discussing results, students gave meaning to their observations. In this stage we found explicit links between properties of substances and micro level structures or the term ‘…molecule’ (figure 4). An example is stated in the quote in section 3.1.3 where ‘hydrophilic’ is linked to O-H or N-H bonds in a molecule.

3.2.2. stages of the design project in which no SPR was identified
Performing the experiment and building and testing of the prototypes were the more hands-on stages of the design project. In these stages no SPR was identified.

4. CONCLUSIONS

The aim of this explorative study was to investigate how students’ structure-property reasoning could be characterized during engagement in this specific design activity. Furthermore, we looked at the link between the expressed SPR at different stages of the design process.

In answer to our first research question, we can state that students’ expressions of SPR emerged within one of 3 ways:

- As a link between structural features and substances
- As a link between the term ‘…molecule’ and property of a substance
- As a link between molecular structures or characteristic moieties and the property of a substance.

Almost all of the SPR coded fragments were found in the data of group 1. In group 2 the only expression of SPR was found in an annotated drawing on one of the worksheets (figure 4). This confirms the added value of using multiple sources of data when looking at students’ thinking during design activities (Stammes et al., 2023).

In answer to our second research question, we saw that SPR was expressed in stages of the design activity in which students gave meaning to their test results and when they generated new ideas. These are processes similar to evaluation, synthesis and structure reformulation in the FBS framework. In these stages students were stimulated to provide explanations and employed evaluative thinking, divergent and subsequent convergent thinking as seen in engineering design (Guzey & Jung, 2021). The function, which states the design requirements was never a topic of debate amongst students.

The project ‘Green bubble soap’ can be used to investigate students’ SPR. The next step will be to use the described method on a larger scale in the context of a professional learning community. By measuring in different classrooms, we can investigate to what extend our results are transferable to other settings and do a more sophisticated analysis of the expressed SPR. Furthermore, with a broader dataset we can closely look into ways to characterise SPR within the FBS framework processes and how it can guide design thinking and thinking about complex systems. By gaining more insight in the way students use this type of reasoning during a design activity we can look at ways to integrate chemical engineering in multidisciplinary design activities in secondary education.

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