Supporting information

Teaching and assessing systems thinking in first-year chemistry

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Alignment with Chemistry themes

The topic of surfactants used in the systems thinking activities aligned to physical and organic chemistry themes covered in the general first-year chemistry module taught at the University of Pretoria. Table 1 shows the alignment of the activities with Physical chemistry themes, which include types of mixtures, physical and chemical properties of substances, intermolecular forces, salts and solubility, acid-base chemistry, and reaction rates. Table 2 shows the alignment of the activities with Organic chemistry themes, which include hybridization and bonding, skeletal structures, isomers, hydrocarbons, fractional distillation, functional groups, and organic reactions. The new chemistry knowledge was introduced to students at the end of the first-year general chemistry module, ensuring that they have relevant prior knowledge before engaging in the systems thinking activities. Students' application of the chemistry knowledge of surfactants formed a core component of Prior Knowledge Quiz 1 and Practical activity 1. The systems knowledge taught in the Surfactant Lesson-Video 3 connected these chemistry themes to society, economy, and environment. Practical activity 1 contained elements of systems knowledge, whereas Systems Knowledge Quiz 2 and Practical activity 2 were primarily based on the systems knowledge of the anionic surfactant, Linear Alkylbenzene Sulfonate (LAS).

Table 1. Physical Chemistry themes aligned with the surfactant (LAS) systems thinking activities

Chemistry Theme	Chemistry Knowledge	Systems knowledge
Homogenous and Heterogeneous Mixtures	The polarity of oil, water, and LAS	• How surfactants work in laundry detergents to remove oil and dirt particles from clothing in the presence of water (emergent behavior)
	The density of oil and water	
Physical properties of substances	Amphiphilic structure of LAS	• Use of LAS in sanitizers and its ability to destroy the lipid-bilayer of Covid -19
	Surface tension	• How surfactants cause foaming
	Concentration	• LAS at non-cytotoxic concentrations and colon cancer • Critical Micelle Concentration and Foaming • Lethal concentration (LC_{50}) and Ecotoxicity • LAS concentration and Biodegradation
	Solubility of LAS and long chain hydrocarbons	• LAS in wastewater absorbed by crops and in the drinking water of rural areas • Bioavailability and sorption into organic matter
Chemical properties of substances	Acidity and basicity (pH) of LAS	• Ecotoxicity of LAS
Intermolecular Forces	London dispersion forces	• The energy required in fractional distillation
	Dipole-dipole IM forces	
Ionic salts and solubility	Inorganic salts (phosphates,	• Biodegradation

	sulfates)	• Eutrophication
Acid-base chemistry	Neutralization with NaOH	• Industrial manufacture of LAS
	Conjugate acid-base pairs	• Biosurfactants
Rates of reaction	Modified Platinum Catalysts	• Platinum reserves in South Africa • Hazards of Heavy metals
	Selectivity	• Waste • Detergency Performance • Market demand and consumption
	Yield	• Large-scale production of LAS

Table 2. Organic Chemistry themes aligned with the surfactant (LAS) systems thinking activities

Organic Chemistry	Chemistry Knowledge	Systems knowledge
Hybridization and bonding	Saturation of hydrocarbons Bond rotation and energy barriers	
Skeletal structures	IUPAC naming	
Isomers	Branched alkyl benzene sulfonates (BAS)	• Foaming • Detergency power
Hydrocarbons	Alkane chain length	• Cytotoxicity
Fractional distillation	The boiling point of crude oil fractions Intermolecular forces Volatility The molar mass of LAS	• Fossil fuels • Non-renewable energy • CO2 emissions and global warming
Functional groups	Alkanes Alkenes Aromatics Sulfonic acid	
Organic reactions	Dehydrogenation	• Industrial manufacture • Modified and unmodified Platinum Catalysts
	Alkylation with benzene	• Carcinogenic reagents
	Sulfonation	• Acid rain • Acid spill • Corrosive reagents
	Synthesis	• Principles of green chemistry • Atom economy • Waste reduction • Renewable feedstock • Safer solvents • Pollution prevention • Biodegradability • Energy efficiency

Design Principles and Justifications

Several design principles were considered for the systems thinking activities. These principles aligned with the seven constructivist principles of practice to ensure that the process of learning is as important as the content, to create opportunities for active learning, to connect new knowledge with students' prior knowledge, to guide students to discover key elements of the topic of surfactants, scaffolding, to encourage group work, co-operative learning and language interaction (Donald, Lazarus, & Moolla, 2014). Enabling opportunities in the classroom for students to connect new knowledge with their prior knowledge, ensuring that the teaching material is meaningful, and allowing students to make their own decisions are core to meaningful learning. (Bretz, 2001). Novak draws strongly onto Ausubel's theory in his theory of education which states that "meaningful learning underlies the constructive integration of thinking, feeling, and acting, leading to human empowerment for commitment and responsibility."(Bretz, 2001) It is also important to reduce the cognitive load experienced by students throughout the activities by ensuring teaching materials are structured to minimize the "chunks" of information that can be processed by students working memory. Our working memories can hold up to four "chunks" of information and if this is overloaded, students will be at risk of not understanding the content and learning will be ineffective (Centre for Education Statistics and Evaluation, 2017). Group work and cooperative learning can allow students to share their cognitive load with their peers. Careful sequencing of new content and scaffolding of activities can also reduce the "chunks" of information that students have to process in their working memories at a time.

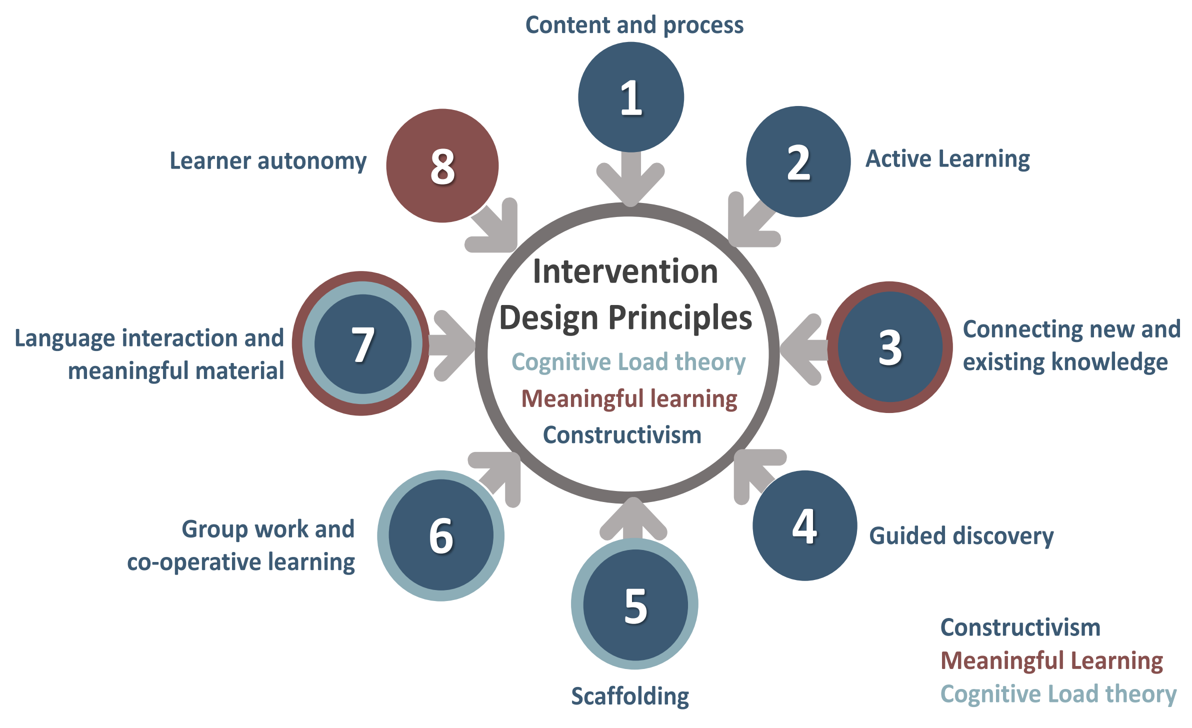

Figure 1. Intervention design principles based on constructivism (dark blue), cognitive load theory (light blue), and meaningful learning (red)

These design principles encourage active agency, metacognition, the social construction of knowledge, and working with tools of cognition that are important factors during the active construction and reconstruction of knowledge by students as they progress to higher levels of understanding (Donald et al., 2014). These principles stem from work done by Piaget (cognitive constructivism) Vygotsky (social constructivism), Bruner (discovery learning), Ausubel (knowledge assimilation), and Novak (human constructivism and meaningful learning.) These design principles were incorporated into different elements of the systems thinking activities as discussed below.

Content and Process

The process of learning is as important as the content so that students can comprehend the underlying structure of a topic through understanding the relationships between the core concepts (Donald et al., 2014). In chemistry, multilevel thinking is required to link macro and sub-micro concepts together with symbolic knowledge to interpret chemical phenomena (Taber, 2013). The ability to link the relevant chemistry concepts for making comparisons, translations, and judgments is key to developing a deeper understanding (Vachliotis, Salta, & Tzougraki, 2021). Therefore, students' deeper understanding is encouraged if they can apply their multi-level thinking to understand the relationships between chemistry concepts as opposed to rote learning facts and information. However, students should be taught certain skills and learning strategies that will enable them to interlink chemistry concepts. The process of developing systems thinking skills in students can contribute significantly to improving their deeper understanding of chemistry concepts (Vachliotis et al., 2021). Systems thinking can incite meaningful understanding as students apply multilevel reasoning to analyze chemistry knowledge which can potentially enable them to see the hidden dimensions such as patterns and interrelationships that are not easily seen (Ben-Zvi-Assaraf & Orion, 2010; Pazicni & Flynn, 2019). Therefore, in the Introduction to Systems Thinking- Video 1 students are introduced to systems thinking and its significance in our society today. This is to enable students to recognize the important role that chemistry can play in future sustainability. Students are also taught about concept mapping as a powerful learning strategy to better visualize the content and identify core concepts and relationships that make up the structure of a topic. A Core Chemistry Concept Map is discussed at the end of the Surfactant Lesson- Video 3 to guide students in their conceptual understanding of the chemistry involved in surfactants, such as LAS.

Active learning

An active learning approach guides learners to construct their knowledge through “action, reflection, abstraction and application” (Swan, 2004). Active learning promotes deeper engagement with chemistry content as students increase their ability to engage with higher-order cognitive skills (Freeman et al., 2014;

Summerton, Hurst, & Clark, 2018). Piaget's theory of cognitive constructivism highlights that students are constantly engaging in the active construction of knowledge onto pre-existing cognitive structures (Piaget, 1971). Cognitive development and learning are not passive, even during instruction, students should always be challenged cognitively within their zone of proximal development (Donald et al., 2014; L. S Vygotsky, 1980). During the quizzes and practical activities, students are encouraged to work actively together in groups to submit answers onto an online platform, where answers should be matched and chosen from a dropdown menu, a jumbled sentence should be completed and an area clicked on a picture (hot spot image) to identify the correct concept or linking word on a given concept map. In Practical Activity 2, a partial SOCME diagram should be expanded by adding new concepts, and linking words, connections, and subsystems onto PowerPoint.

Connecting new with existing knowledge

David Ausubel described that meaningful learning occurs when new knowledge is purposefully linked to existing knowledge frameworks. (Ausubel, 1968) This is put nicely by Bruner in his statement that learning is about "knowing how to use what you already know to go beyond what you already think" (Bruner, 1985). Students should recall what they know when they complete Prior Knowledge Quiz 1 to prepare them for the new chemistry learning about surfactants. As students engage with the unfamiliar chemistry of how surfactants work, they might experience discomfort as a result of their cognitive conflict to make connections to their existing knowledge. This is where guidance or mediation from group facilitators or educators is important to assist students in their zone of proximal development. The Core Chemistry Concept Map also guides in that regard as it facilitates the process of connecting new knowledge to existing knowledge. This aligns with Novak's statement that concept mapping is powerful for the facilitation of meaningful learning as it serves as a scaffold to help organize and structure new knowledge onto prior knowledge (Novak & Cañas, 2006). Concept maps are also valuable to the educator to understand the process of how students construct meanings as it provides a "window" into a student's mind (Bretz, 2001).

Guided discovery

Students need facilitation so that they can discover key concepts in the conceptual structure of a topic (Donald et al., 2014). This is a powerful learning strategy as students are guided to discuss, reflect and argue about possible solutions to the problems they need to solve with their group members (Donald et al., 2014). This design principle is important to facilitate learning to not only develop students' confidence as they engage in active discussions but to also develop their higher-order cognitive skills. Throughout the systems thinking quizzes and practical activities, students are prompted to engage with each other, conduct their research, and consult the additional resources that are provided, such as the Example SOCME Diagrams or Journal Articles and Media Reports. Guided discovery is process oriented and promotes active learning, self-directive learning, and reflective thinking in students (Noer, Gunowibowo, & Triana, 2020). Student's reflective learning can be improved as they work on contextual problems that make them curious to learn more, which can be facilitated with guided discovery learning (Noer et al., 2020). Therefore, the case studies and literature chosen for discussion in Surfactant Lesson- Video 3 are centered around relevant issues that students can relate to in South Africa. This includes pollution in the Hennops river and the laundry detergent in rivers near the rural community in the Balfour village in the Eastern Cape. Reflective thinking can also improve when students get an opportunity to conclude the problem under study (Noer et al., 2020). Therefore, the Take Home Message- Video 4 is shown so that students can answer questions from the Self-reflection Questionnaire to conclude by explaining the most important chemical properties and behavior of LAS that contribute to its value in our economy, its health impacts on our society, and environmental consequences throughout its life cycle from crude oil to ultimate biodegradation. It also asks students to reflect on how the chemistry and engineering of LAS can be altered to ensure sustainable manufacturing, minimal environmental consequences, and safe but effective detergents for household use. Students' ability to reflect on their learning allows them to step back and visualize the system of LAS with its complex interconnections and to think critically about its implications and its role in society, the environment, and the economy. According to Mezirow, "to think critically means to adopt a more reflective attitude toward human experience". It is this reflective attitude together with questioning norms and practices that put critical thinkers in a position to take sustainable action (Taimur & Sattar, 2019).

Scaffolding

Learning is scaffolded throughout the systems thinking activities to reduce the cognitive load that students might experience. Students are guided throughout the content and activities to learn chemistry and systems thinking skills sequentially from the known to the unknown. This is done with guidance from facilitators, the use of visualization tools, and the structuring of systems thinking skills. Therefore, the learning is structured sequentially to build new chemistry knowledge into students' relevant Chemistry prior knowledge. The systems thinking skills are scaffolded after an initial understanding of the chemistry is developed. They are then prompted to apply their analysis skills followed by their synthesis skills, this is where the scaffold is removed, and students are asked to apply both their analysis and synthesis skills. They are then asked to reflect on their learning, where an attitude of taking ownership and taking sustainable action is prompted. SOCMEs can provide an effective solution for cognitive overload, as a zoom-in and out strategy can be used during instruction to direct one's attention towards concepts and connections within a specific subsystem (Pazicni & Flynn, 2019). Students are guided throughout the activities to gradually zoom out of the chemistry with the use of concept maps and SOCME diagrams. The learning starts from a Core Chemistry Concept Map, onto which new concepts are added to link the molecular and system level in different Expanded Concept Maps to visualize the concepts and connections within the societal, environmental, and economic subsystems. The perspective from which the system is viewed changes to a system level in the Partial SOCME, where the Chemistry concepts are now "hidden". The final SOCME is then created after the expansion of the Partial SOCME to demonstrate systems thinking skills to show new concepts, connections, subsystems, subsystem boundaries, and predictions. Novak recommended that concept maps used as skeleton frameworks or "scaffolds" containing 20 concepts can be expanded to 50 -60 concepts to encourage high cognitive performance. (Novak & Cañas, 2006)

Groupwork and co-operative learning

The jig-saw cooperative design encourages the interdependence between group members and reduces the cognitive load associated with the system under consideration. It also incorporates mediation between peers, which aligns with Vygotsky and Bruner's theory and promotes active agency (Donald et al., 2014, p. 114). Cooperation between peers enables cognitive conflict during knowledge assimilation and encourages students to adapt their thinking, which aids in problem-solving as their quality of thinking about moral and social issues improves (Donald et al., 2014, pp. 72-77). Students' cognitive development depends on their experiences gained from interacting with the physical and social world, to become active agents in constructing knowledge "from the inside out and outside in" (Donald et al., 2014, p. 106). Hoffman asserted that visualizations can "facilitate individual or social thinking processes in situations that are too complex to be coped with exclusively by internal cognitive means" (Aubrecht et al., 2019; Hoffmann, 2011). Therefore, the construction of SOCMEs with limited boundaries together with collaboration can ultimately reduce the cognitive load experienced during the systems thinking activities. For group work to be sufficient, it must have clear outcomes, support social interaction and be well organized and monitored so that all group members participate actively to accomplish the group's common goals (Donald et al., 2014, p. 109). To encourage active participation in the systems thinking activities each group member in their home group has a dedicated role, such as the group facilitator, a presenter/recorder, and a strategy analyst/researcher each with respective tasks as shown in table 3 below.

Table 3: Group Roles for each home group throughout the Systems Thinking Activities

Group Facilitator	Group Presenter/Recorder	Group Strategy Analyst/Researcher
• Asks questions to the instructor • Responsible for group work • Makes sure all voices are heard • Encourages group members • Ensures active participation during practical sessions	• Must share their screen during online group activities • Record the collaborative session • Work on PowerPoint on behalf of the group • Reads the questions before the group engages in discussion	• Takes care of time management • Monitors group interactions and suggests improvements to group dynamics to ensure that the task is completed • Conducts research to find additional information. • Tries to resolve disagreements by researching for more information.

The Introductory Activities can also enhance the group dynamics by taking into consideration the processes of forming, storming, norming, and performing (Tuckman, 1965). The groups can also be organized in such a way to have maximum academic ability per group to ensure each group has a more knowledgeable other that can start conversations regarding possible solutions to the problems. The jig-saw-designed cooperative enables active participation, and language interaction and can enhance students' confidence as they communicate their expert knowledge gained in their subsystem groups with their home groups for the expansion of the SOCME diagram.

Language interaction and meaningful material

Language is an important tool in teaching and learning as knowledge transmits between learners that interact with each other (L. S. Vygotsky, 1964). Learners should be encouraged to interact with language through speaking, reading, presenting, writing, and expressing their views during discussions (Donald et al., 2014, p. 109). In the systems thinking activities learners are encouraged to engage in group discussions to solve problems, express themselves in their group roles, and refine their writing skills as they reflect on their learning in the Self-reflection Questionnaire. The activities are designed in such a way to encourage learners with different group roles to communicate with each other and to express their thoughts to enhance their confidence. For meaningful learning, the language used in the learning materials must be clear and should relate to students' relevant prior knowledge (Novak & Cañas, 2006). The learning and teaching materials were also formulated to reduce cognitive load by keeping slides simple and by ensuring the language are clear in the concept maps and SOCMEs. Another important aspect of meaningful materials is that they must be structured in a suitable sequence to scaffold the learning process to build new knowledge into students' relevant prior knowledge (Novak & Cañas, 2006). This is done by ensuring that students are introduced to what systems thinking and concept mapping is and why it is important, then by asking them to recall prior chemistry knowledge, before learning the new chemistry of surfactants and LAS.

Learner autonomy

For meaningful learning to occur, students must decide to learn meaningfully. As educators, we can indirectly influence the choices learners to make by motivating students to incorporate new meaning into their prior knowledge (Novak & Cañas, 2006). In this way, students are encouraged to learn more meaningfully and not by rote learning, which enables longer retention of new knowledge in their long-term memories (Novak & Cañas, 2006). Incorporating relevance into the Chemistry classroom can already motivate students to choose to learn meaningfully as they recognize the real-world implications of Chemistry in their everyday lives. Systems thinking provides opportunities for students to “connect chemistry with issues that matter to them from local to global levels” which enhances the value of chemistry learning and their motivation (Pazicni & Flynn, 2019). The Prior Knowledge Quiz 1 makes learning relevant by asking students to use their prior knowledge of the properties of oil and water can explain why a surfactant molecule can work in laundry detergents to remove oil and dirt from clothing in the presence of water. Throughout the Surfactant Lesson-

Video 3, the chemistry was made relevant by connecting the use of LAS in sanitizers and laundry detergents and how it has played a role in breaking the bilipid membrane of the Covid-19 virus, how it can be manufactured from our local manufacturer, Sasol, and how it can contribute to foaming in rivers, concerning the Hennops river and our rural communities in South Africa. Students also feel more empowered and motivated to learn when they get to make their own choices. Students are encouraged to make their own choices throughout the activities by choosing their group roles, choosing an SDG that represents them, and using that to introduce themselves to their group members. They also get to choose their subsystem, which might align with their interests, and are free to be creative and choose concepts, linking words and subsystems that they think are relevant to the system based on their prior knowledge and experiences.

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