Supporting information

Development of Systems Thinking in a large first-year chemistry course using a group activity on detergents

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INTERVENTION DESCRIPTION

Contents

A. Context.

The intervention was developed and used for online teaching during the Covid-19 pandemic.[1] The context of this revised intervention occurred in a face-to-face setting in the equivalent second-semester course that consisted of general and introductory organic chemistry. Students alternated between attending a laboratory session and a large class tutorial every week. The activity was conducted towards the end of the semester during two laboratory sessions utilizing the laboratory space for collaborative group work rather than a theatre-style lecture venue typically available for the large class tutorials. Laboratories accommodated 100-150 students each. The students learning was facilitated by teaching assistants in a ratio of 25:1.

B. The schedule.

Students were required to prepare for the first session by watching three interactive videos via the Learning Management System (LMS). This preparation would take about 1 hour. The activities for the first contact session were planned to fit into two of the three hours (Table S-1).

Table S-1: Schedule for Session 1

Time	Activity	Points
10 min	Instructions and formation of home groups	
Home Groups (3 per group)		
5 min	Choose favorite SDGs, group name, group roles, and subsystems	
20 min	Work on Chemistry Quiz	15
15 min	Add to a chemistry concept map	10
10 min	Class reorganizes into subsystem groups	
Subsystem Groups (3 or 4 per group)		
15 min	Share favorite SDGs. Choose group roles. Play the subsystem video clip.	
25 min	Practical activity 1 – linking molecular level to visible level	20
20 min	Draft a concept map – linking visible/local to national/global level.	15

Each student left session 1 with a photo of their subsystem group concept map. They had to redraw and improve on that concept map in preparation for Session 2 two weeks later. The schedule for session 2 is shown in Table S-2.

Table S-2: Schedule for Session 2

Time	Activity	Points
10 min	Instructions	
Home Groups (3 per group)		
30 min	Work on Quiz 2	25
60 min	Work on SOCME – link subsystems, add future predictions	80
20 min	Final video on options to improve sustainability.	

After session 2, the students were tasked to complete a reflection via the LMS.

C. Description of the activities.

Preparation

The course learning management system directed the students to prepare for the activity by watching three videos with “in-video” assessments. The first video, 11 minute duration, introduced the concept of “Systems Thinking” and provided foundational teaching on concept mapping formalisms. The second video, 5 minute duration, zoomed in to the molecular level world of why oil and water do not mix in preparation for the introduction to surfactants in the third video. The third video (30 minutes) provided overview information on the surfactant linear alkyl benzene sulfonate (LAS), its chemical function, its chemical synthesis from an economic perspective (5.5 min), its impact on the environment (4.5 min) and its positive and negative impacts on society (7.5 min). Students had to download the three short excerpts of this informational video to their devices to review one of the relevant sections (economic, environmental, or societal impact) during the activity.

Face-to-Face Session 1

On arrival, teaching assistants divided students into groups of three members, their home group. To assist with the group forming, the members had to consider the SDGs, choose the one that mattered to them the most and give a reason. They also had to select a group name, assign group roles inspired by POGIL (e.g., group manager/timekeeper, scribe, and researcher), and choose a subsystem (economic, environmental, and societal).

The home group’s first assessment task was to complete a quiz that focused their attention on the molecular-level chemistry of LAS (Figure S-1). After that, they had to add visible characteristics of the chemistry to a partial concept map by adding the visible characteristic as a concept and how it links to the chemical property.

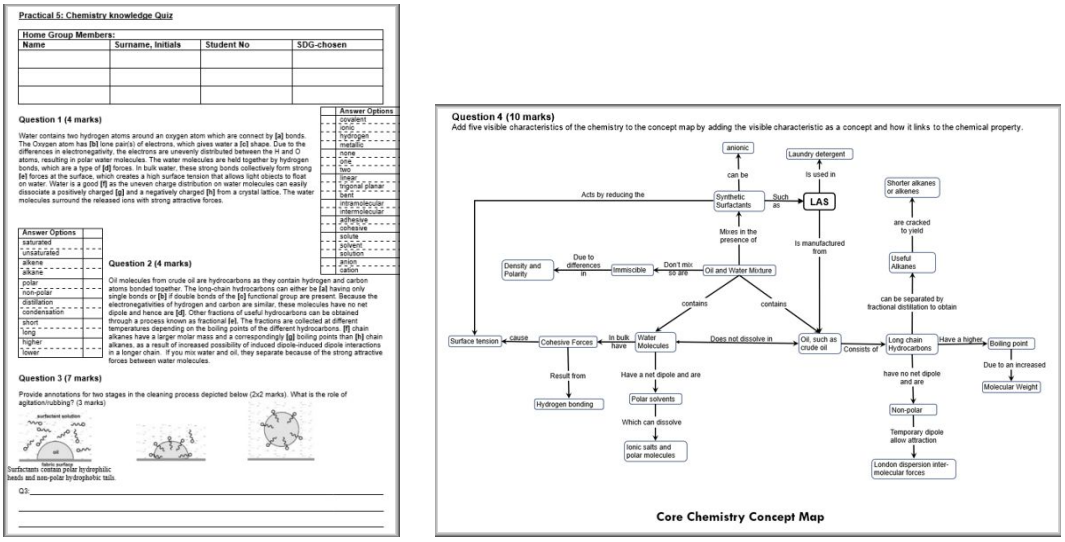
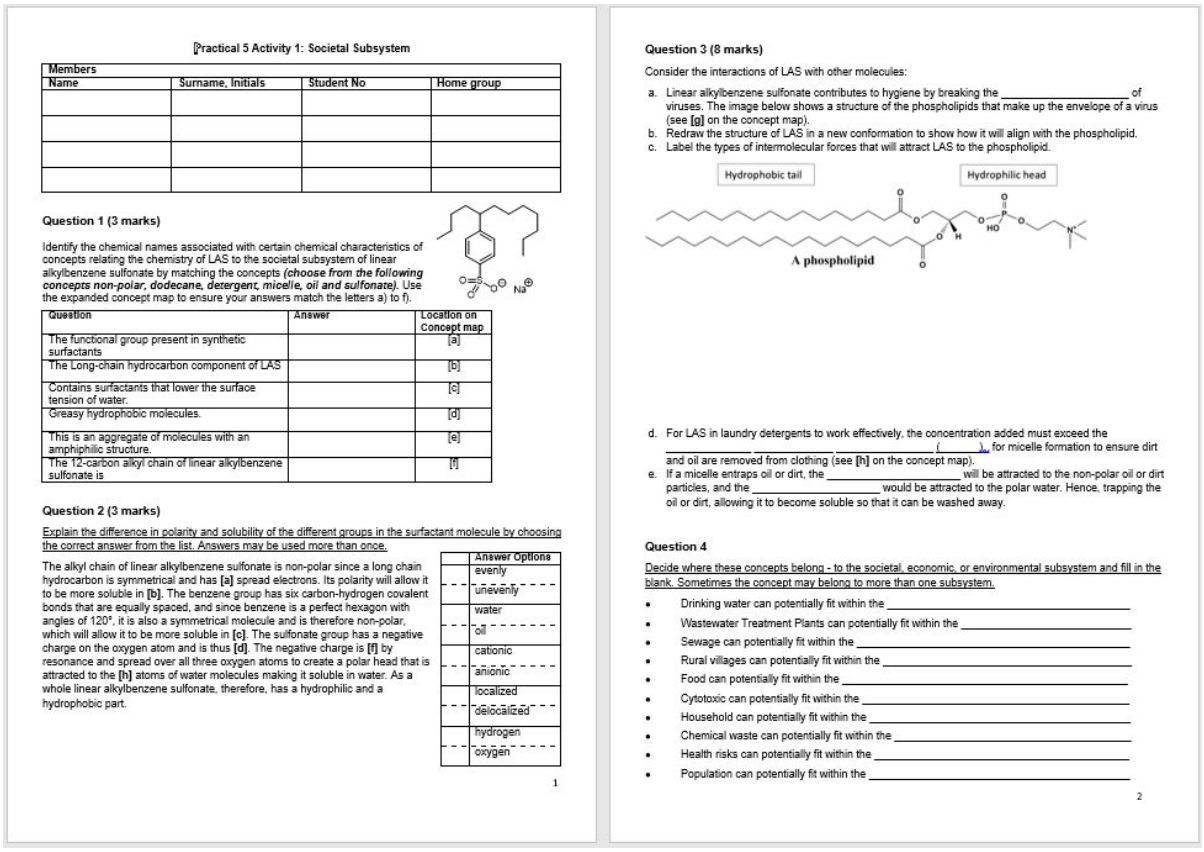


Figure S-1. Home group chemistry knowledge quiz

In line with the jigsaw cooperative learning approach,[2] after completing their home group tasks, the students formed new “subsystem” groups of four with others of the same subsystem. Students introduced themselves to each other in the same manner as for the home groups. They watched the subsystem video clip (5-8 minutes) to refresh the information pertinent to their subsystem that they learned during their preparation. The group then worked on an activity to help them zoom out from the chemistry level to the implications for their subsystem (Figure S-2 and Appendix).



Practical 5 Activity 1: Societal Subsystem

Members			
Name	Surname, Initials	Student No	Home group

Question 1 (3 marks)

Identify the chemical names associated with certain chemical characteristics of concepts relating the chemistry of LAS to the societal subsystem of linear alkylbenzene sulfonate by matching the concepts ***(choose from the following concepts non-polar, dodecane, detergent, micelle, oil and sulfonate)***. Use the expanded concept map to ensure your answers match the letters a) to f).

Question	Answer	Location on Concept map
The functional group present in synthetic surfactants		[a]
The Long-chain hydrocarbon component of LAS		[b]
Contains surfactants that lower the surface tension of water.		[c]
Greasy hydrophobic molecules.		[d]
This is an aggregate of molecules with an amphiphilic structure.		[e]
The 12-carbon alkyl chain of linear alkylbenzene sulfonate is		[f]

Question 2 (3 marks)

Explain the difference in polarity and solubility of the different groups in the surfactant molecule by choosing the correct answer from the list. Answers may be used more than once.

The alkyl chain of linear alkylbenzene sulfonate is non-polar since a long chain hydrocarbon is symmetrical and has **[a]** spread electrons. Its polarity will allow it to be more soluble in **[b]**. The benzene group has six carbon-hydrogen covalent bonds that are equally spaced, and since benzene is a perfect hexagon with angles of 120°, it is also a symmetrical molecule and is therefore non-polar, which will allow it to be more soluble in **[c]**. The sulfonate group has a negative charge on the oxygen atom and is thus **[d]**. The negative charge is **[f]** by resonance and spread over all three oxygen atoms to create a polar head that is attracted to the **[h]** atoms of water molecules making it soluble in water. As a whole linear alkylbenzene sulfonate, therefore, has a hydrophilic and a hydrophobic part.

Answer Options
evenly
unevenly
water
oil
cationic
anionic
localized
delocalized
hydrogen
oxygen

1

Question 3 (8 marks)

Consider the interactions of LAS with other molecules:

a. Linear alkylbenzene sulfonate contributes to hygiene by breaking the _____ of viruses. The image below shows a structure of the phospholipids that make up the envelope of a virus (see **[g]** on the concept map).
b. Redraw the structure of LAS in a new conformation to show how it will align with the phospholipid.
c. Label the types of intermolecular forces that will attract LAS to the phospholipid.

Hydrophobic tail | Hydrophilic head

A phospholipid

d. For LAS in laundry detergents to work effectively, the concentration added must exceed the _____ ( ), for micelle formation to ensure dirt and oil are removed from clothing (see **[h]** on the concept map).
e. If a micelle entraps oil or dirt, the _____ will be attracted to the non-polar oil or dirt particles, and the _____ would be attracted to the polar water. Hence, trapping the oil or dirt, allowing it to become soluble so that it can be washed away.

Question 4

Decide where these concepts belong - to the societal, economic, or environmental subsystem and fill in the blank. Sometimes the concept may belong to more than one subsystem.

- Drinking water can potentially fit within the _____
- Wastewater Treatment Plants can potentially fit within the _____
- Sewage can potentially fit within the _____
- Rural villages can potentially fit within the _____
- Food can potentially fit within the _____
- Cytotoxic can potentially fit within the _____
- Household can potentially fit within the _____
- Chemical waste can potentially fit within the _____
- Health risks can potentially fit within the _____
- Population can potentially fit within the _____

2

Question 5 (6 marks)

The chemistry concept map was extended to include some of the impact of the **chemistry of LAS** on the **societal subsystem**.

i. Add the concepts and relationships **[a]** to **[h]**.
ii. Read the propositions in this extended concept map linking to **concepts in bold**. Note any improvements you wish to make.
iii. Formulate the relationships between concepts for arrows **[j]** and **[k]** indicating the nature of the intermolecular forces (ion-dipole, London dispersion, dipole-dipole).
iv. Highlight the concept (block) that is responsible for spread of linear alkylbenzene sulfonate into society and the environment.

3

Question 6 (15 marks)

Draft a new concept map – linking visible/local level concepts (incidents/actions) associated with the societal subsystem to national/global level concepts (effects).

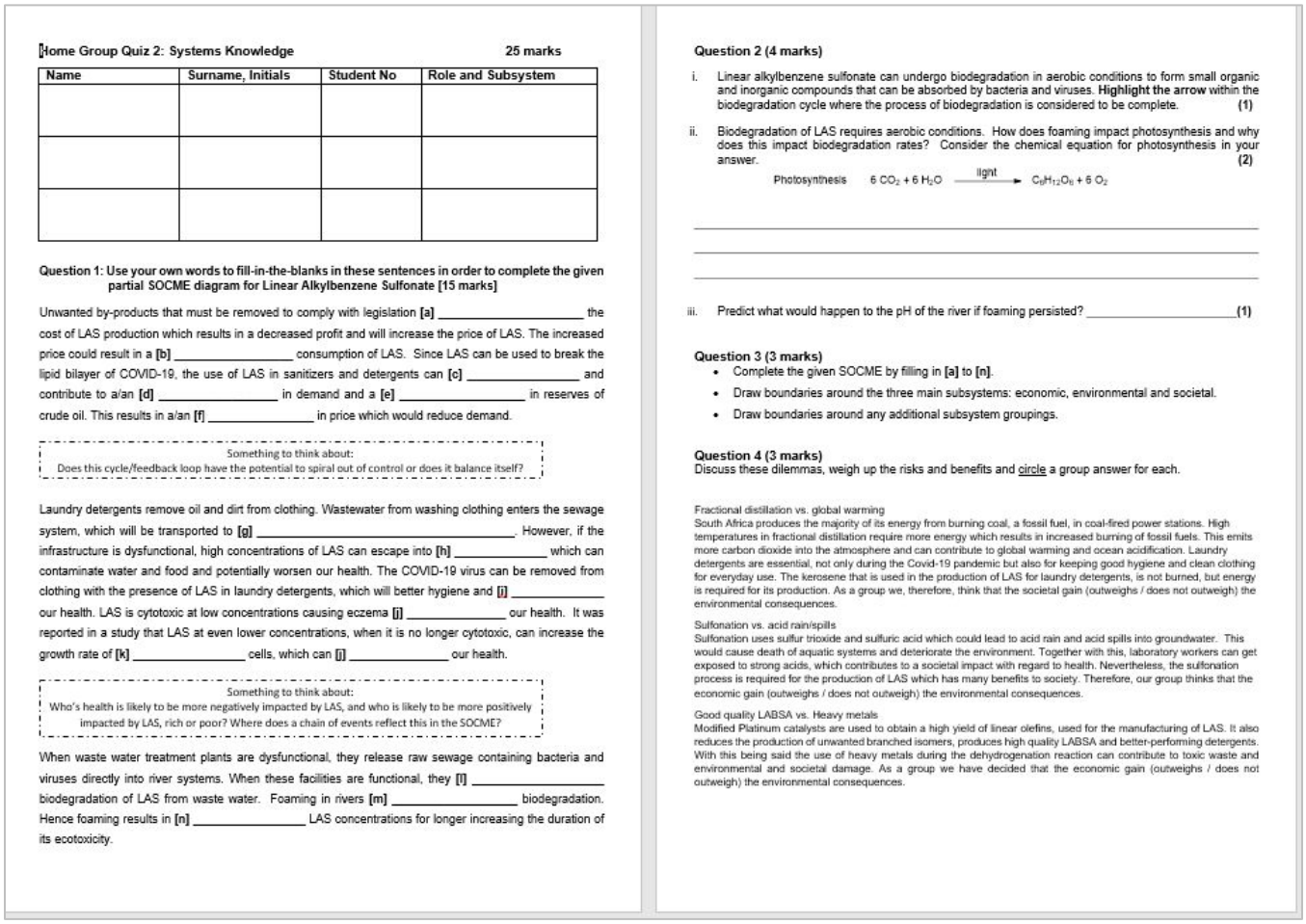
1. Start with the concepts of LAS, health benefits, health risks, waste water. Connect these concepts to each other.
2. Then be creative and expand your concept map by branching to more concepts as you think of the impact of LAS on society and what makes it better or worse and how society's handling of LAS can have impact.
3. Then consider your answers to question 3 above and propose links from the societal subsystem to the economic and environmental subsystems.
4. Each member should take a copy of this concept map to serve as a foundation for their preparation for prac 6.

Figure S-2. Societal subsystem group activity.

The first contact session concluded with the subsystem groups drafting a new concept map to elicit further connections from what they had learned to other subsystems and broader impacts. Before submitting their work, group members took a photograph of their concept map. This concept map had to be redrawn and expanded individually in preparation for the second contact session.

Face-to-Face Session 2

At the start of the second session, students convened in their home groups and worked together on a systems knowledge quiz to integrate their subsystem perspectives. The task was also designed to stimulate critical thinking as students had to engage with scenarios that had tradeoffs. For example, the use of heavy metals for efficient synthesis of LAS versus avoiding these and producing a lower quality product with a slower biodegradation (Figure S-3.



Home Group Quiz 2: Systems Knowledge **25 marks**

Name	Surname, Initials	Student No	Role and Subsystem

Question 1: Use your own words to fill-in-the-blanks in these sentences in order to complete the given partial SOCME diagram for Linear Alkylbenzene Sulfonate [15 marks]

Unwanted by-products that must be removed to comply with legislation **[a]** _____ the cost of LAS production which results in a decreased profit and will increase the price of LAS. The increased price could result in a **[b]** _____ consumption of LAS. Since LAS can be used to break the lipid bilayer of COVID-19, the use of LAS in sanitizers and detergents can **[c]** _____ and contribute to a/an **[d]** _____ in demand and a **[e]** _____ in reserves of crude oil. This results in a/an **[f]** _____ in price which would reduce demand.

Something to think about:
Does this cycle/feedback loop have the potential to spiral out of control or does it balance itself?

Laundry detergents remove oil and dirt from clothing. Wastewater from washing clothing enters the sewage system, which will be transported to **[g]** _____. However, if the infrastructure is dysfunctional, high concentrations of LAS can escape into **[h]** _____ which can contaminate water and food and potentially worsen our health. The COVID-19 virus can be removed from clothing with the presence of LAS in laundry detergents, which will better hygiene and **[i]** _____ our health. LAS is cytotoxic at low concentrations causing eczema **[j]** _____ our health. It was reported in a study that LAS at even lower concentrations, when it is no longer cytotoxic, can increase the growth rate of **[k]** _____ cells, which can **[j]** _____ our health.

Something to think about:
Who's health is likely to be more negatively impacted by LAS, and who is likely to be more positively impacted by LAS, rich or poor? Where does a chain of events reflect this in the SOCME?

When waste water treatment plants are dysfunctional, they release raw sewage containing bacteria and viruses directly into river systems. When these facilities are functional, they **[l]** _____ biodegradation of LAS from waste water. Foaming in rivers **[m]** _____ biodegradation. Hence foaming results in **[n]** _____ LAS concentrations for longer increasing the duration of its ecotoxicity.

Question 2 (4 marks)

i. Linear alkylbenzene sulfonate can undergo biodegradation in aerobic conditions to form small organic and inorganic compounds that can be absorbed by bacteria and viruses. **Highlight the arrow** within the biodegradation cycle where the process of biodegradation is considered to be complete. **(1)**

ii. Biodegradation of LAS requires aerobic conditions. How does foaming impact photosynthesis and why does this impact biodegradation rates? Consider the chemical equation for photosynthesis in your answer. **(2)**

Photosynthesis $6\,CO_2 + 6\,H_2O \xrightarrow{light} C_6H_{12}O_6 + 6\,O_2$

iii. Predict what would happen to the pH of the river if foaming persisted? _____ **(1)**

Question 3 (3 marks)

- Complete the given SOCME by filling in **[a]** to **[n]**.
- Draw boundaries around the three main subsystems: economic, environmental and societal.
- Draw boundaries around any additional subsystem groupings.

Question 4 (3 marks)
Discuss these dilemmas, weigh up the risks and benefits and circle a group answer for each.

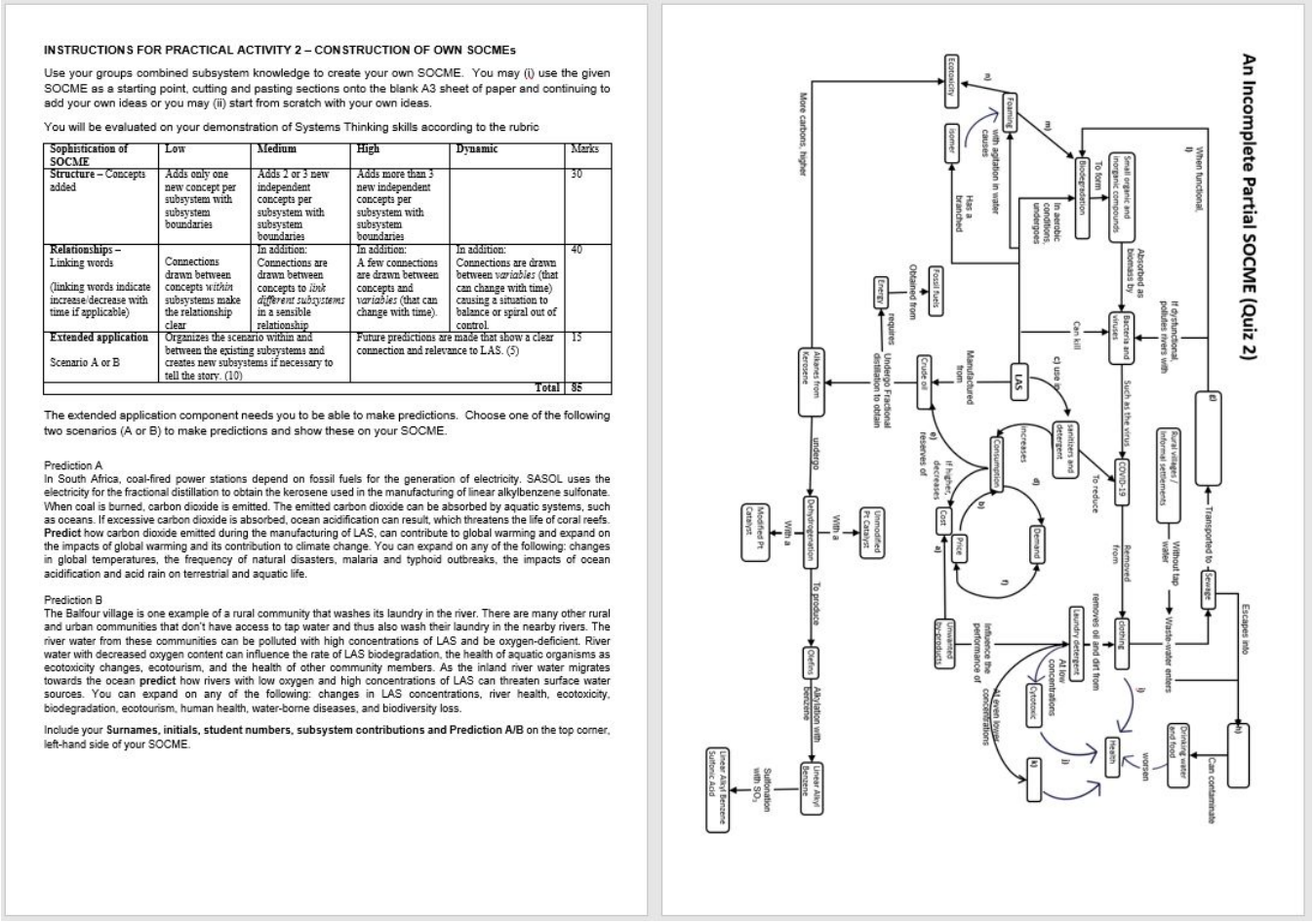
Fractional distillation vs. global warming
South Africa produces the majority of its energy from burning coal, a fossil fuel, in coal-fired power stations. High temperatures in fractional distillation require more energy which results in increased burning of fossil fuels. This emits more carbon dioxide into the atmosphere and can contribute to global warming and ocean acidification. Laundry detergents are essential, not only during the Covid-19 pandemic but also for keeping good hygiene and clean clothing for everyday use. The kerosene that is used in the production of LAS for laundry detergents, is not burned, but energy is required for its production. As a group we, therefore, think that the societal gain (outweighs / does not outweigh) the environmental consequences.

Sulfonation vs. acid rain/spills
Sulfonation uses sulfur trioxide and sulfuric acid which could lead to acid rain and acid spills into groundwater. This would cause death of aquatic systems and deteriorate the environment. Together with this, laboratory workers can get exposed to strong acids, which contributes to a societal impact with regard to health. Nevertheless, the sulfonation process is required for the production of LAS which has many benefits to society. Therefore, our group thinks that the economic gain (outweighs / does not outweigh) the environmental consequences.

Good quality LABSA vs. Heavy metals
Modified Platinum catalysts are used to obtain a high yield of linear olefins, used for the manufacturing of LAS. It also reduces the production of unwanted branched isomers, produces high quality LABSA and better-performing detergents. With this being said the use of heavy metals during the dehydrogenation reaction can contribute to toxic waste and environmental and societal damage. As a group we have decided that the economic gain (outweighs / does not outweigh) the environmental consequences.

Figure S-3. Home group systems knowledge quiz

To this stage, the tasks of sessions 1 and 2 served to develop a broad understanding of the system from the molecular level chemistry to its macroscopic effects and broader impacts on the economy, environment and society through engaging them in various systems thinking dimensions. This scaffolded development prepared them for the primary goal of the assignment: to demonstrate their systems thinking by constructing a System Oriented Concept Map Extension (SOCME) diagram. The home groups were allowed to start their SOCME with a blank page or use the partial SOCME provided as a template. To stimulate their temporal thinking, they were challenged to consider the future long-term impacts of LAS given a scenario and to depict the outcomes on their SOCMEs (Figure S-4). The groups were allocated 60 minutes to complete this task.



INSTRUCTIONS FOR PRACTICAL ACTIVITY 2 – CONSTRUCTION OF OWN SOCMEs

Use your groups combined subsystem knowledge to create your own SOCME. You may (i) use the given SOCME as a starting point, cutting and pasting sections onto the blank A3 sheet of paper and continuing to add your own ideas or you may (ii) start from scratch with your own ideas.

You will be evaluated on your demonstration of Systems Thinking skills according to the rubric

Sophistication of SOCME	Low	Medium	High	Dynamic	Marks
Structure – Concepts added	Adds only one new concept per subsystem with subsystem boundaries	Adds 2 or 3 new independent concepts per subsystem with subsystem boundaries	Adds more than 3 new independent concepts per subsystem with subsystem boundaries		30
Relationships – Linking words (linking words indicate increase/decrease with time if applicable)	Connections drawn between concepts *within* subsystems make the relationship clear	In addition: Connections are drawn between concepts to *link different subsystems* in a sensible relationship	In addition: A few connections are drawn between concepts and *variables* (that can change with time).	In addition: Connections are drawn between *variables* (that can change with time) causing a situation to balance or spiral out of control.	40
Extended application Scenario A or B	Organizes the scenario within and between the existing subsystems and creates new subsystems if necessary to tell the story. (10)		Future predictions are made that show a clear connection and relevance to LAS. (5)		15
				Total	**85**

The extended application component needs you to be able to make predictions. Choose one of the following two scenarios (A or B) to make predictions and show these on your SOCME.

Prediction A
In South Africa, coal-fired power stations depend on fossil fuels for the generation of electricity. SASOL uses the electricity for the fractional distillation to obtain the kerosene used in the manufacturing of linear alkylbenzene sulfonate. When coal is burned, carbon dioxide is emitted. The emitted carbon dioxide can be absorbed by aquatic systems, such as oceans. If excessive carbon dioxide is absorbed, ocean acidification can result, which threatens the life of coral reefs. **Predict** how carbon dioxide emitted during the manufacturing of LAS, can contribute to global warming and expand on the impacts of global warming and its contribution to climate change. You can expand on any of the following: changes in global temperatures, the frequency of natural disasters, malaria and typhoid outbreaks, the impacts of ocean acidification and acid rain on terrestrial and aquatic life.

Prediction B
The Balfour village is one example of a rural community that washes its laundry in the river. There are many other rural and urban communities that don't have access to tap water and thus also wash their laundry in the nearby rivers. The river water from these communities can be polluted with high concentrations of LAS and be oxygen-deficient. River water with decreased oxygen content can influence the rate of LAS biodegradation, the health of aquatic organisms as ecotoxicity changes, ecotourism, and the health of other community members. As the inland river water migrates towards the ocean **predict** how rivers with low oxygen and high concentrations of LAS can threaten surface water sources. You can expand on any of the following: changes in LAS concentrations, river health, ecotoxicity, biodegradation, ecotourism, human health, water-borne diseases, and biodiversity loss.

Include your **Surnames, initials, student numbers, subsystem contributions and Prediction A/B** on the top corner, left-hand side of your SOCME.

Figure S-4. Home group activity instructions for the construction of a group SOCME.

The session concluded with the general playing of a video that shared some chemistry research into developing more sustainable surfactants. Since not everyone can afford the more environmentally friendly products, they were challenged to wash their clothing less often or to experiment with using lower doses of laundry detergents to reduce their consumption of LAS.

Post-activity reflections

Depending on the students allocation to a particular laboratory session, they had from one week to two-and-a-half weeks to complete a reflection on their learning experience. The reflection prompts were:

1. What did you learn from practicals 5 and 6? You can mention specific knowledge, understanding, or skills and was it interesting or useful?
2. What aspects did you like or enjoy about these practicals?
3. How could aspects of these practicals that you disliked be improved?
4. If sustainability matters, who should take responsibility for it and how?
5. Do you think it would be good to
   i. continue with the two systems thinking pracs,
   ii. combine them into just one practical session and have one lab based prac, or
   iii. replace both systems thinking pracs with two wet-lab pracs?

   Please explain your choice.

D. Constructive criticism and subsequent modifications to the intervention design

Responses to students' reflections on Question 3, their answers to Question 5 above, and the feedback from the teaching assistants was studied for criticism to make future modifications. Students and TA's requested more time for the various tasks and suggested using the entire three hours. Students asked for opportunities to do experiments that illustrated the chemistry they were learning, e.g. micelle formation or foaming. TA's suggested that it would be helpful if students were re-convened in subsystem groups at the start of the second session for improved continuity. Students said that the partial SOCME provided to scaffold their own SOCME construction was too full and represented ideas that they had come up with independently, denying them the opportunity to be rewarded for their independent thinking. Some students felt so strongly about the importance of taking sustainable action due to the intervention that they were concerned that not all their classmates had taken the message as seriously.

As a result of this feedback, the intervention design was adjusted for improved learning as follows:

1. Time was increased to 3 hours per contact session.
2. A wet laboratory component was introduced at the start of session 1. The mixed drops of cooking oil and water determined the amount of laundry detergent required to dissolve the oil.
3. The students started session 2 in their subsystem groups to consolidate their individual subsystem concept map development and empower them to rejoin their home groups as subsystem experts.
4. The partial SOCME provided in session 2 was simplified with fewer scaffolding concepts provided to allow the students to contribute more.
5. Students were given a pledge card to complete while watching the final video of tips to improve sustainability. This gave them an opportunity to commit to making any personal change for a more sustainable future. These pledge cards were taken home as a reminder.

In addition, with fewer concepts included in the provided partial SOCME, the rubric was adjusted to challenge groups to add more concepts to each subsystem. It reflected the possibility of differential grading within a group if a subsystem was under-developed relative to the others, indicating a deficient contribution from one of the group members (Figure S-5).

Sophistication of SOCME	**Low**	**Medium**	**High**	**Dynamic**	Marks
Structure – Concepts added	Adds only three new concept per subsystem with subsystem boundaries	Adds 4 or 5 new independent concepts per subsystem with subsystem boundaries	Adds more than 5 new independent concepts per subsystem with subsystem boundaries		30
Relationships – Linking words (linking words indicate increase/decrease with time if applicable)	Connections drawn between concepts *within* subsystems make	In addition: Connections are drawn between concepts to *link different subsystems*	In addition: A few connections are drawn between concepts and *variables* (that can change with time).	In addition: Connections are drawn between *variables* (that can change with time) causing a situation to	40

	the relationship clear	in a sensible relationship		balance or spiral out of control.	
Application of Scenario A or B	Organizes the scenario within and between the existing subsystems and creates new subsystems if necessary to tell the story. (10)		Future predictions are made that show a clear connection and relevance to LAS. (5)		15
				Total	**85**

Figure S-5. Revised rubric for the assessment of group SOCMEs.

E. Changes to the intervention compared to the published design.

The intervention design has been published.[5] Initially it was implemented online due to the Covid-19 pandemic. For this study, the students met face-to-face. In addition, the number of students participating was much larger (1039) than in the pilot study. Minor adjustments were made to the quizzes for the face-to-face setting. A major adjustment to the rubric was required to facilitate assessment for the large enrolment. The rubric used is included in Figure S-4.

REFERENCES

1. Reynders, M., Pilcher, L. A. and Potgieter, M. Teaching and Assessing Systems Thinking in First-Year Chemistry. *J. Chem. Educ.* **2023**, 100, 1357-1365.
2. Theobald, E. J.; Eddy, S. L.; Grunspan, D. Z.; Wiggins, B. L.; Crowe, A. J. Student Perception of Group Dynamics Predicts Individual Performance: Comfort and Equity Matter. *PLoS One* **2017**, *12* (7). https://doi.org/10.1371/journal.pone.0181336.

Appendix: Full intervention worksheets

Practical 5: Chemistry knowledge Quiz 1

Home Group				
Name	**Surname, Initials**	**Student No**	**SDG #**	**Role and Subsystem**

a) Each group member must choose an SDG that you identify with most and tell your group why.
b) Allocate group roles.
- The **scribe** fills in the worksheet,
- The **researcher** looks up information when needed
- The **timekeeper** ensures the group spends the appropriate time on each question so the worksheet can be completed.

c) Choose a group name.
d) Choose one group member for each subsystem: Economic, Environmental and Societal.

The 17 sustainable development goals (SDGs)
1: No Poverty
2: Zero Hunger
3: Good Health and Well-being
4: Quality Education
5: Gender Equality
6: Clean Water and Sanitation
7: Affordable and Clean Energy
8: Decent Work and Economic Growth
9: Industry, Innovation and Infrastructure
10: Reduced Inequality
11: Sustainable Cities and Communities
12: Responsible Consumption and Production
13: Climate Action
14: Life Below Water
15: Life on Land
16: Peace and Justice Strong Institutions
17: Partnerships to achieve the Goal

Question 1 (4 marks)

Water contains two hydrogen atoms around an oxygen atom which are connect by **[a]** bonds. The Oxygen atom has **[b]** lone pair(s) of electrons, which gives water a **[c]** shape. Due to the differences in electronegativity, the electrons are unevenly distributed between the H and O atoms, resulting in polar water molecules. The water molecules are held together by hydrogen bonds, which are a type of **[d]** forces. In bulk water, these strong bonds collectively form strong **[e]** forces at the surface, which creates a high surface tension that allows light objects to float on water. Water is a good **[f]** as the uneven charge distribution on water molecules can easily dissociate a positively charged **[g]** and a negatively charged **[h]** from a crystal lattice**.** The water molecules surround the released ions with strong attractive forces.

	Answer Options
	covalent
	ionic
	hydrogen
	metallic
	none
	one
	two
	linear
	trigonal planar
	bent
	intramolecular
	intermolecular
	adhesive
	cohesive
	solute
	solvent
	solution
	anion
	cation

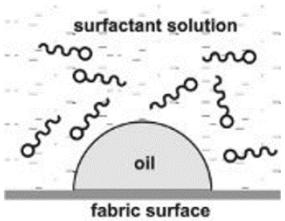
Question 2 (4 marks)

Answer Options	
saturated	
unsaturated	
alkane	
alkene	
polar	
non-polar	
distillation	
condensation	
short	
long	
higher	
lower	

Oil molecules from crude oil are hydrocarbons as they contain hydrogen and carbon atoms bonded together. The long-chain hydrocarbons can either be **[a]** having only single bonds or **[b]** if double bonds of the **[c]** functional group are present. Because the electronegativities of hydrogen and carbon are similar, these molecules have no net dipole and hence are **[d]**. Other fractions of useful hydrocarbons can be obtained through a process known as fractional **[e].** The fractions are collected at different temperatures depending on the boiling points of the different hydrocarbons. **[f]** chain alkanes have a larger molar mass and a correspondingly **[g]** boiling points than **[h]** chain alkanes, as a result of increased possibility of induced dipole-induced dipole interactions in a longer chain. If you mix water and oil, they separate because of the strong attractive forces between water molecules.

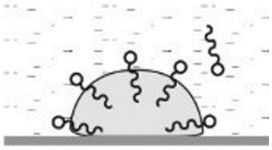
Question 3 (7 marks)

Provide annotations for stages **II** and **III** in the cleaning process depicted below (2x2 marks).

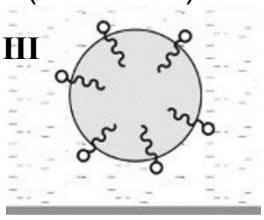


Surfactants contain polar hydrophilic heads and non-polar hydrophobic tails.

II



III



_____ _____

_____ _____

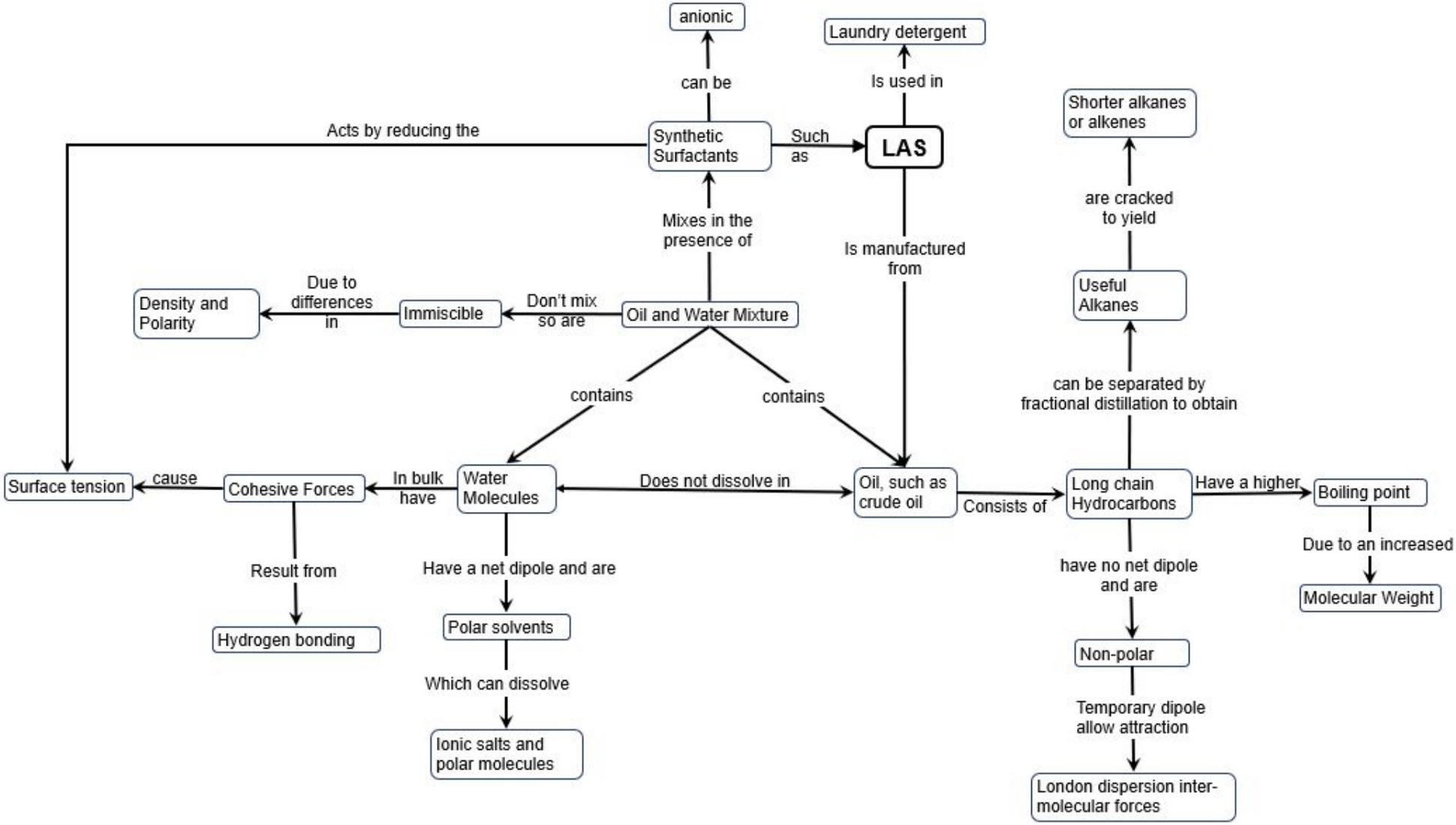
At what stage is agitation/rubbing necessary and why? (3 marks)

_____

_____

Question 4 (10 marks)

Add five visible characteristics of the chemistry to the concept map by adding the visible characteristic as a concept and how it links to the chemical property.



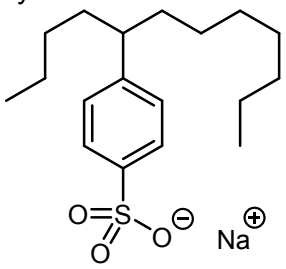
Core Chemistry Concept Map

Practical 5 Activity 1: Economic Subsystem

Members			
Name	**Surname, Initials**	**Student No**	**Home group**

Question 1 (6 marks)

The structure of Linear alkylbenzene sulfonate is shown below (LAS). Answer the following questions to relate the chemical properties and chemical behaviour of LAS to the economic subsystem.



Match the characteristics to the chemical name/concept. ***Choose from the following concepts and relationships: Dodecane, Kerosene, Alkene, Benzene, Sulfonate, Sodium Hydroxide, strong, weak.*** *Some answers are used twice.* Use the expanded concept map to ensure your answers match the letters a) to h)

Question	**Answer**	**Location on Concept map**
The functional group that makes LAS a synthetic surfactant.		[a]
Long-chain hydrocarbon in LAS.		[b]
Obtained after the fractional distillation of crude oil.		[c]
Olefins with the …… functional group are unsaturated		[d]
Is an aromatic, but also carcinogenic reactant used in the industrial manufacture of LAS.		[e]
LAS is manufactured by neutralization with		[f]
Sodium Hydroxide is a …. base with pH > 7.		[g]
[a] groups are a … conjugate base of sulfonic acid.		[h]
Is aromatic, planar with bond angles of 120 degrees; all carbons are sp^2 hybridized.		
Has trigonal planar carbons with a large energy barrier to rotation.		
Has tetrahedral carbons with freely rotating sigma bonds and is insoluble in water.		
Is collected higher up in the fractional distillation column in comparison to diesel oil and waxes		

Remember to complete the expanded concept map on page 3.

Question 2 (5 marks)

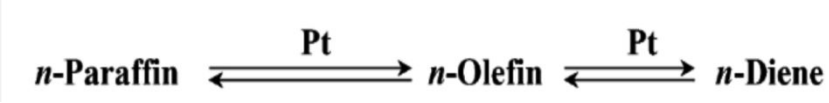
Use the expanded concept map to ensure your answers match the letters [i], to [n].

i. Choose the correct answers from the dropdown list about the primary feedstock used for the manufacturing of linear alkylbenzene sulfonate.

Sasol and other industries that manufacture Linear alkylbenzene sulfonate depend on the raw material **[w]** as a **[x]** feedstock. Usually, 75% of the linear alkanes which are extracted from kerosene are used in the production of Linear alkylbenzene. Kerosene has a boiling point between 175 °C and 325 °C. However, the boiling point of kerosene is **[i]** in comparison to the boiling points of other fractions such as diesel, oil, waxes, and bitumen. The compounds in Kerosene have fewer carbons than molecules in the **[y]** boiling fractions, which, therefore **[j]** its molecular weight and the strength of the **[k]** intermolecular forces. Hence, less energy is required to disrupt attractive **[z]** forces for vaporization to occur.

	Answer Options
	LAB
	crude oil
	renewable
	non-renewable
	higher
	lower
	increases
	decreases
	dipole-dipole
	London dispersion
	intermolecular
	intramolecular
	hydrogenation
	dehydrogenation
	modified
	unmodified
	increase
	reduce

ii. Select the correct answers for the following paragraph that also describes this diagram shown below:



To obtain olefins (alkenes) from linear paraffin (alkanes), a/an **[l]** reaction should occur with a/an **[m]** platinum catalyst to obtain high yields of olefins with high selectivity to **[n]** unwanted by-products (dienes).

Question 3

Decide where these concepts belong - to the societal, economic, or environmental subsystem and fill in the blank. Sometimes the concept may belong to more than one subsystem.

Heavy metals can potentially be within the _____

Platinum Exports can potentially be within the _____

Job creation can potentially be within the _____

Greenhouse gasses can potentially be within _____

Carcinogenic can potentially be within the _____

Chemical waste can potentially be within the _____

Health risks can potentially be within the _____

Oil spills can potentially be within the _____

Fossil fuels can potentially be within the _____

Global warming can potentially be within the _____

Question 4 (9 marks)

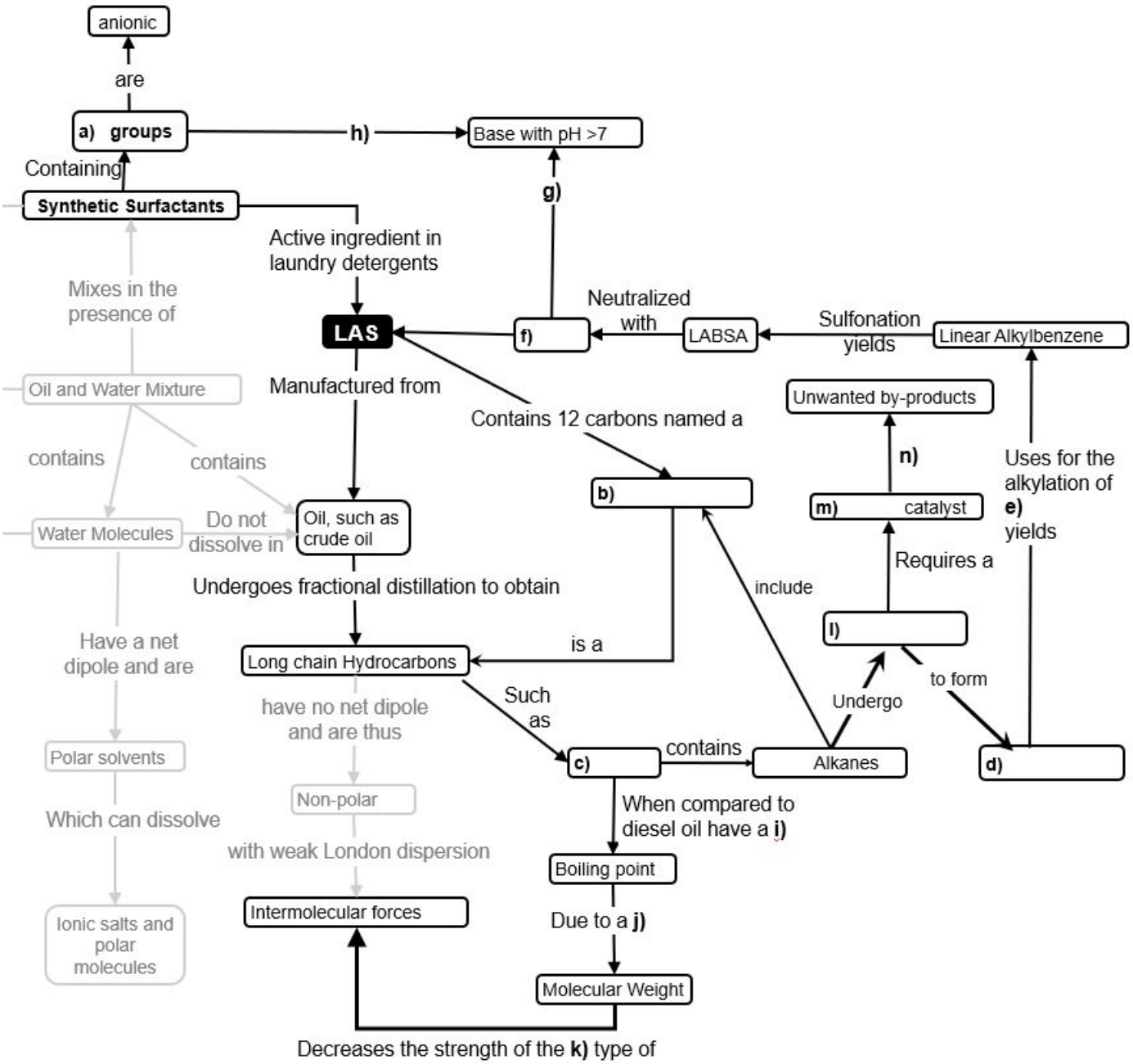
The chemistry concept map was extended to include some of the impact of the **chemistry of LAS** on the manufacturing process within the **economic subsystem**.

i. Add the concepts and relationships **[a]** to **[n]**.

ii. Read the propositions in this extended concept map linking to **concepts in bold**. Make any improvements to improve the links.

iii. Highlight the concept (block) that influences the activation energy of a reaction and could therefore reduce time and the energy that the reaction requires for synthesis in the industrial manufacturing process.

iv. Highlight the relationship in the manufacturing process that poses a risk to the environment in terms of acid spills and acid rain.



Question 5 (15 marks)

Draft a new concept map – linking visible/local level concepts (incidents/actions) associated with the economic subsystem to national/global level concepts (effects).

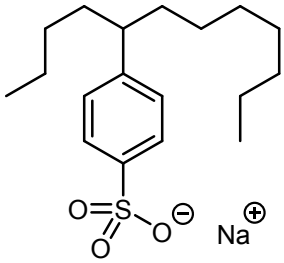
1. Start with the concepts of LAS, manufacturing process, profit, costs, benefits. Connect these concepts to each other.
2. Then be creative and expand your concept map by branching to more concepts as you think of the impact of LAS on the economy and what makes it better or worse.
3. Then consider your answers to question 3 above and propose links from the economic subsystem to the societal and environmental subsystems.
4. Each member should take a copy of this concept map to serve as a foundation for their preparation for prac 6.

Practical 5 Activity 1: Environmental Subsystem

Members			
Name	**Surname, Initials**	**Student No**	**Home group**

Question 1 (5 marks)

Alkanes aren't soluble in water, however, Linear Alkylbenzene Sulfonate (LAS) containing a long chain of 12 carbons, is soluble in water. The structure of a LAS molecule can be seen below.



Complete the sentences to explain the solubility properties of LAS.
(the options can be chosen more than once)

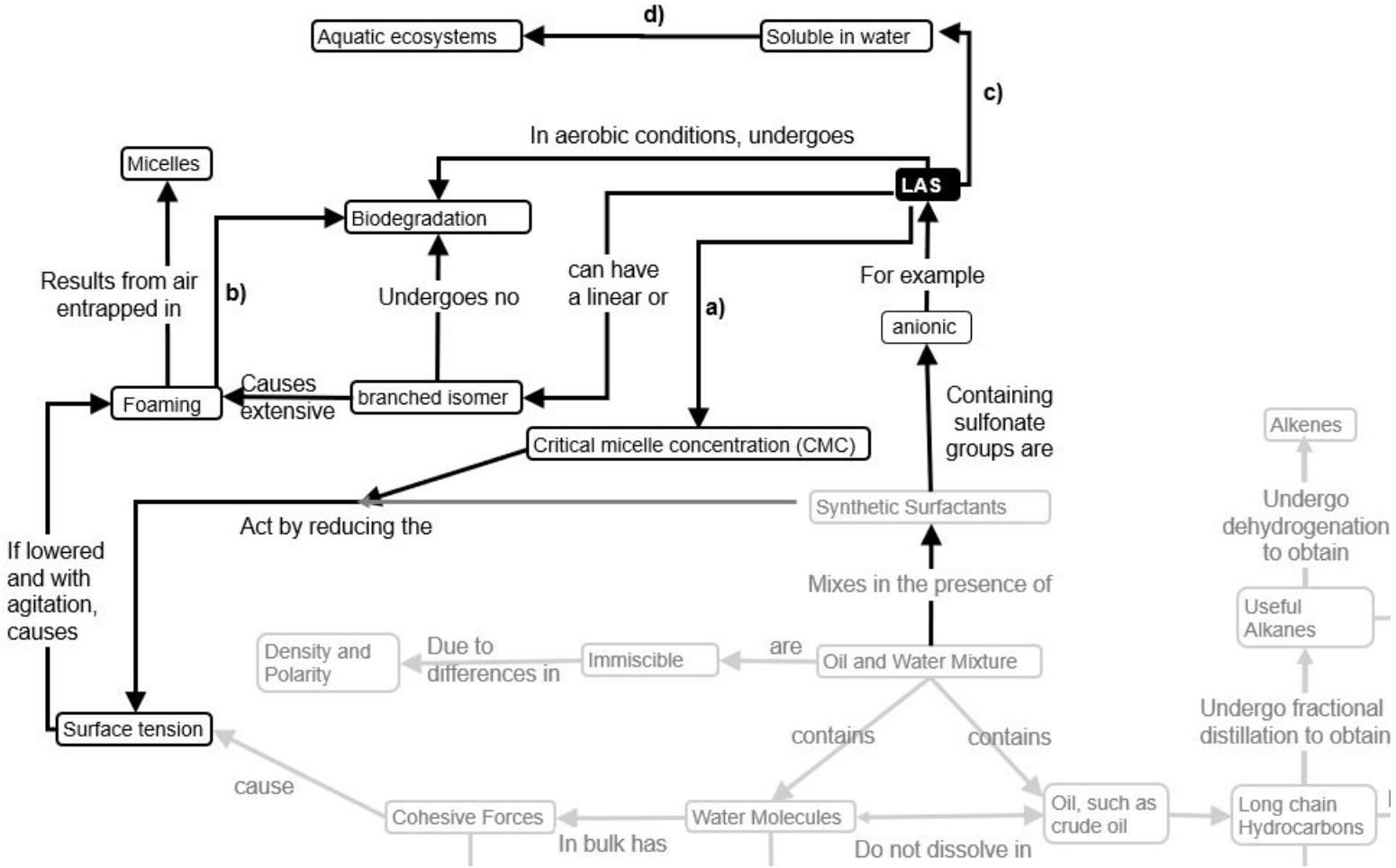
An example of a long-chain hydrocarbon that contains 12 carbons is known as a **[a].** This alkane is **[b]** because of its symmetry and **[c]** spread electrons, making it **[d]** in water. Linear alkylbenzene sulfonate is soluble in water, even though it contains two alkyl substituents, a/an **[e]** group (8 carbons) and a/an **[f]** group (4 carbons). The benzene group has many carbon-hydrogen bonds that are equally spaced, and since benzene is a perfect hexagon with angles of 120°, it is also symmetrical and is, therefore **[g],** which makes it **[h]** soluble in water. To explain the high solubility of linear alkylbenzene sulfonate we can look *at* **[i]** such as sodium chloride, sodium sulfonate, and sodium linear alkylbenzene sulfonate, that can **[j]** into cations and anions. The ion-dipole attractive forces cause the water molecules to surround the sodium cations and the sulfonate anions in linear alkylbenzene sulfonate and make it soluble in water. It is the high solubility of linear alkylbenzene sulfonate that makes it an environmental concern as it can easily be transported in aquatic ecosystems and terrestrial ecosystems where it can be absorbed by aquatic life and food crops.

	Answer Options
	decane
	dodecane
	polar
	non-polar
	evenly
	unevenly
	soluble
	insoluble
	butyl
	octyl
	propyl
	poorly
	very
	metallic compounds
	ionic salts
	ionise
	dissociate

Question 2 (5 marks)

The chemistry concept map was extended to include some of the impact of the **chemistry of LAS** on the **environmental subsystem**.

v. Read the propositions in this extended concept map linking to **concepts in bold**. Note any improvements you wish to make.
vi. Add relationships between concepts for arrows **[a]** to **[d]**.
vii. Highlight the concept (block) that is responsible for changing the amount of linear alkylbenzene sulfonate over time.



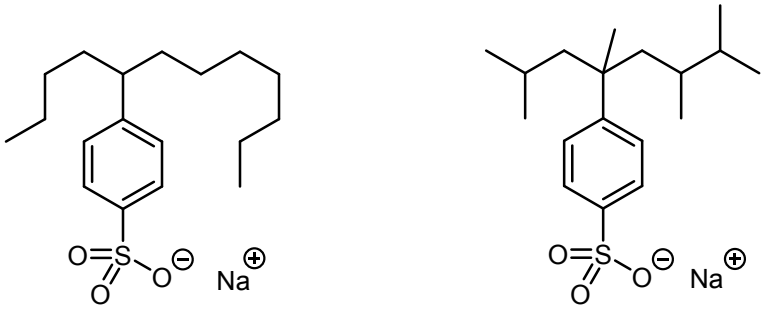
Question 3 (4 marks)

Surfactants are surface-active agents that can allow gas to mix with a liquid, a liquid to mix with a liquid, and a liquid to mix with a solid by lowering the surface tension of the liquid. To explain the process behind the formation of foam, order the following statements (from 1 to 5). Use the concept map as a guide.

	Foaming can block sunlight, prevent photosynthesis in river plants and decrease the available oxygen in the river.
	LAS has an amphiphilic structure, with a hydrophilic head that is attracted to water and a hydrophobic tail is attracted to air.
	As the concentration of LAS exceeds the critical micelle concentration, the surface tension of the water will reduce significantly.
	The surfactant micelles of LAS entrap air and results in more foaming as agitation increase.
	With a reduced surface tension, LAS causes air to mix with water upon agitation

Question 4 (4 marks)

Branched alkyl benzene sulfonates (BAS) as indicated on the right of the diagram below, have a greater detergency power and produce more foaming, however in the 1960's BAS was phased out as excessive foaming and inability to biodegrade resulted in environmental concerns.



i. **Select the answer that describes an isomer.**

A. One of two or more atoms of a chemical element with the same atomic number and nearly identical chemical behaviour but with different atomic masses and physical properties

B. Contain the same number of atoms for each element, but the atomic arrangement differs. Despite having the same molecular formula, the physical properties of each molecule may differ

C. A compound belonging to a series of compounds with similar chemical properties with the same general formula, differing from each other by a repeating unit.

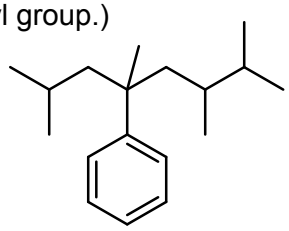
D. Contain the same number of atoms for each element, but the atomic arrangement differs. Despite having a different molecular formula, the physical properties of each molecule are the same

ii. **Identify the IUPAC name of the benzene pre-cursor of BAS as shown below.**
(Hint: the benzene substituent is known as a phenyl group.)

A. 2,3,5,7-tetramethyl- 5-phenyloctane

B. 4-phenyl-2,4,6,7-tetramethyloctane

C. 2,4,6,7-tetramethyl-4-phenyloctane



Question 5 (2 marks)

Anionic surfactants with longer chain lengths have a higher detergency power but more severe environmental impact.
Which concept is described in each case? Choose between lethal concentration, surface tension, ecotoxicity and solubility.

Question	Answer
A. Longer carbon chains chain lengths increase the …….. of surfactants.	
B. Longer chains, together with branched chains, decrease the ……. of LAS which allows it to settle into soils, absorb into organic matter, and can be absorbed by aquatic organisms.	
C. Longer carbon chains exhibit lower critical micelle concentrations; therefore, LAS with longer carbon chains reduce the ……. of water at lower concentrations and allow the surfactant to cause extensive foaming.	
D. The ……. of LAS with a12-carbon linear alkyl chain, required to kill 50% of the *Pimephales promelas* fish species, is 3.2 mg/l.	

Question 6

Decide where these concepts belong - to the societal, economic, or environmental subsystem and fill in the blank. Sometimes the concept may belong to more than one subsystem.

- Drinking water can potentially fit within the _____
- Wastewater Treatment Plants can potentially fit within the _____
- Sewage can potentially fit within the _____
- Rural villages can potentially fit within the _____
- Food can potentially fit within the _____
- Cytotoxic can potentially fit within the _____
- Household can potentially fit within the _____
- Chemical waste can potentially fit within the _____
- Health risks can potentially fit within the _____
- Population can potentially fit within the _____

Question 7 (15 marks)

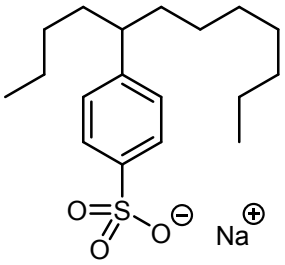
Draft a new concept map – linking visible/local level concepts (incidents/actions) associated with the environmental subsystem to national/global level concepts (effects).

5. Start with the concepts of LAS, foaming, biodegradation, ecotoxicity. Connect these concepts to each other.
6. Then be creative and add more concepts as you think of the impact of LAS on the environment and what makes it better or worse.
7. Then consider your answers to question 6 above and propose links from the environmental subsystem to the societal and economic subsystems.
8. Each member should take a copy of this concept map to serve as a foundation for their preparation for prac 6.

Practical 5 Activity 1: Societal Subsystem

Members			
Name	Surname, Initials	Student No	Home group

Question 1 (3 marks)



Identify the chemical names associated with certain chemical characteristics of concepts relating the chemistry of LAS to the societal subsystem of linear alkylbenzene sulfonate by matching the concepts ***(choose from the following concepts non-polar, dodecane, detergent, micelle, oil and sulfonate).*** Use the expanded concept map to ensure your answers match the letters a) to f).

Question	**Answer**	**Location on Concept map**
The functional group present in synthetic surfactants		[a]
The Long-chain hydrocarbon component of LAS		[b]
Contains surfactants that lower the surface tension of water.		[c]
Greasy hydrophobic molecules.		[d]
This is an aggregate of molecules with an amphiphilic structure.		[e]
The 12-carbon alkyl chain of linear alkylbenzene sulfonate is		[f]

	Answer Options
	evenly
	unevenly
	water
	oil
	cationic
	anionic
	localized
	delocalized
	hydrogen
	oxygen

Question 2 (3 marks)

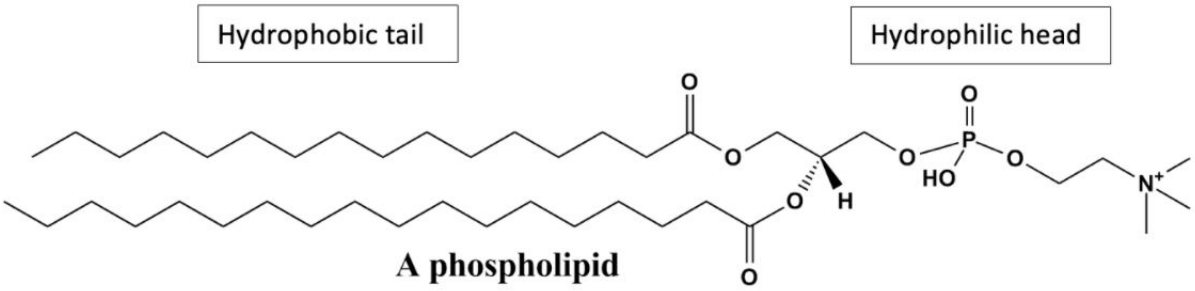
<u>Explain the difference in polarity and solubility of the different groups in the surfactant molecule by choosing the correct answer from the list. Answers may be used more than once.</u>

The alkyl chain of linear alkylbenzene sulfonate is non-polar since a long chain hydrocarbon is symmetrical and has **[a]** spread electrons. Its polarity will allow it to be more soluble in **[b].** The benzene group has six carbon-hydrogen covalent bonds that are equally spaced, and since benzene is a perfect hexagon with angles of 120°, it is also a symmetrical molecule and is therefore non-polar, which will allow it to be more soluble in **[c]**. The sulfonate group has a negative charge on the oxygen atom and is thus **[d]**. The negative charge is **[f]** by resonance and spread over all three oxygen atoms to create a polar head that is attracted to the **[h]** atoms of water molecules making it soluble in water. As a whole linear alkylbenzene sulfonate, therefore, has a hydrophilic and a hydrophobic part.

Question 3 (8 marks)

Consider the interactions of LAS with other molecules:

a. Linear alkylbenzene sulfonate contributes to hygiene by breaking the _____ of viruses. The image below shows a structure of the phospholipids that make up the envelope of a virus (see **[g]** on the concept map).
b. Redraw the structure of LAS in a new conformation to show how it will align with the phospholipid.
c. Label the types of intermolecular forces that will attract LAS to the phospholipid.



A phospholipid

d. For LAS in laundry detergents to work effectively, the concentration added must exceed the _____ _____ _____ (_____) for micelle formation to ensure dirt and oil are removed from clothing (see **[h]** on the concept map).
e. If a micelle entraps oil or dirt, the _____ will be attracted to the non-polar oil or dirt particles, and the _____ would be attracted to the polar water. Hence, trapping the oil or dirt, allowing it to become soluble so that it can be washed away.

Question 4

<u>Decide where these concepts belong - to the societal, economic, or environmental subsystem and fill in the blank. Sometimes the concept may belong to more than one subsystem.</u>

- Drinking water can potentially fit within the _____
- Wastewater Treatment Plants can potentially fit within the _____
- Sewage can potentially fit within the _____
- Rural villages can potentially fit within the _____
- Food can potentially fit within the _____
- Cytotoxic can potentially fit within the _____
- Household can potentially fit within the _____
- Chemical waste can potentially fit within the _____
- Health risks can potentially fit within the _____
- Population can potentially fit within the _____

Question 5 (6 marks)

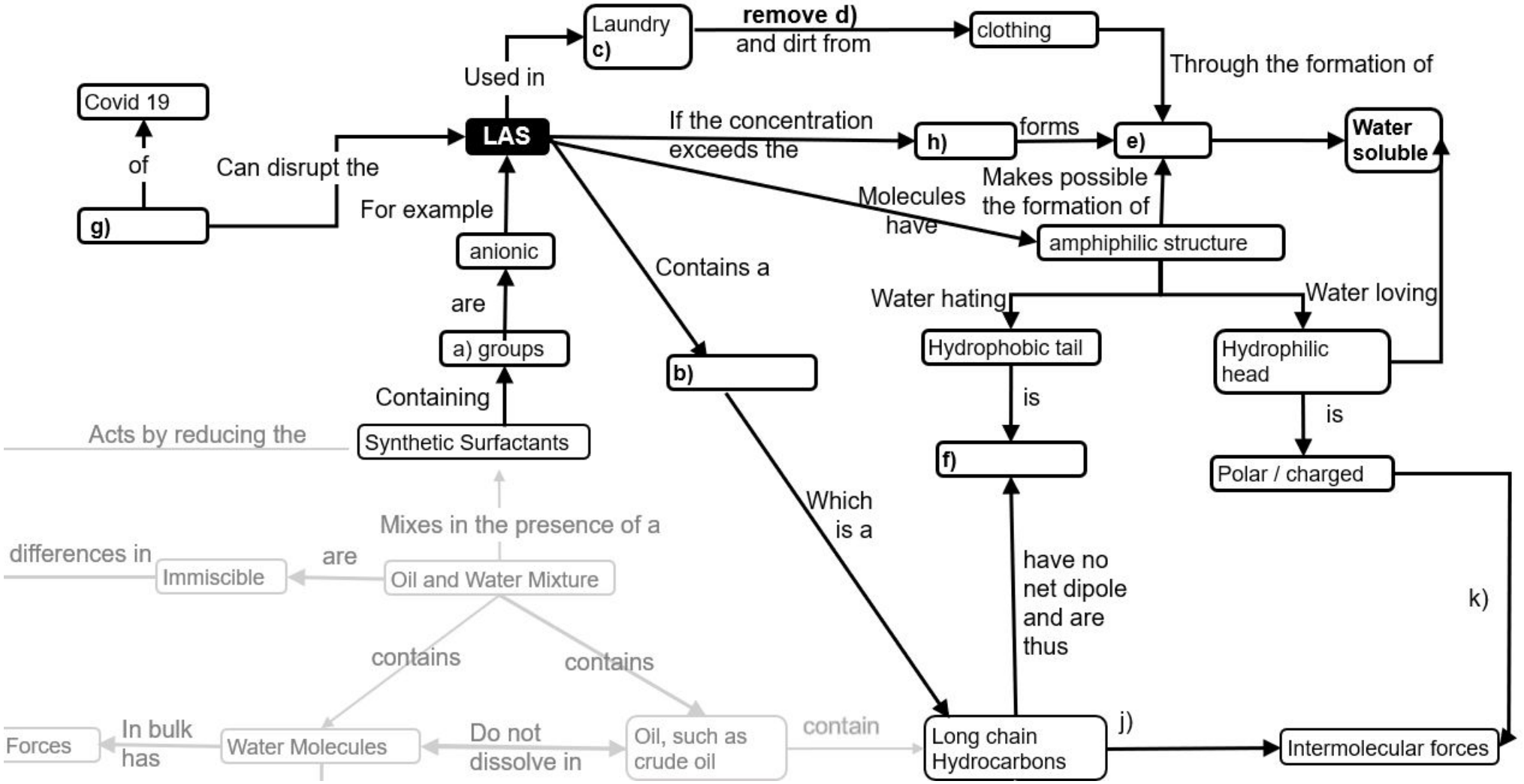
The chemistry concept map was extended to include some of the impact of the **chemistry of LAS** on the **societal subsystem**.

viii. Add the concepts and relationships **[a]** to **[h]**.

ix. Read the propositions in this extended concept map linking to **concepts in bold**. Note any improvements you wish to make.

x. Formulate the relationships between concepts for arrows **[j]** and **[k]** indicating the nature of the intermolecular forces (ion-dipole, London dispersion, dipole-dipole).

xi. Highlight the concept (block) that is responsible for spread of linear alkylbenzene sulfonate into society and the environment.


Laundry
c)
remove d)
and dirt from
clothing
Through the formation of
Used in
Covid 19
of
g)
Can disrupt the
LAS
If the concentration
exceeds the
h)
forms
e)
Water
soluble
Molecules
have
Makes possible
the formation of
amphiphilic structure
For example
anionic
Contains a
are
a) groups
b)
Water hating
Water loving
Hydrophobic tail
Hydrophilic
head
Containing
Synthetic Surfactants
Acts by reducing the
is
is
f)
Polar / charged
Which
is a
Mixes in the presence of a
differences in
Immiscible
are
Oil and Water Mixture
have no
net dipole
and are
thus
k)
contains
contains
Forces
In bulk
has
Water Molecules
Do not
dissolve in
Oil, such as
crude oil
contain
Long chain
Hydrocarbons
j)
Intermolecular forces

Question 6 (15 marks)

Draft a new concept map – linking visible/local level concepts (incidents/actions) associated with the societal subsystem to national/global level concepts (effects).

9. Start with the concepts of LAS, health benefits, health risks, waste water. Connect these concepts to each other.
10. Then be creative and expand your concept map by branching to more concepts as you think of the impact of LAS on society and what makes it better or worse and how society's handling of LAS can have impact.
11. Then consider your answers to question 3 above and propose links from the societal subsystem to the economic and environmental subsystems.
12. Each member should take a copy of this concept map to serve as a foundation for their preparation for prac 6.

Home Group Quiz 2: Systems Knowledge **25 marks**

Name	Surname, Initials	Student No	Role and Subsystem

Question 1: Use your own words to fill-in-the-blanks in these sentences in order to complete the given partial SOCME diagram for Linear Alkylbenzene Sulfonate [15 marks]

Unwanted by-products that must be removed to comply with legislation **[a]** _____ the cost of LAS production which results in a decreased profit and will increase the price of LAS. The increased price could result in a **[b]** _____ consumption of LAS. Since LAS can be used to break the lipid bilayer of COVID-19, the use of LAS in sanitizers and detergents can **[c]** _____ and contribute to a/an **[d]** _____ in demand and a **[e]** _____ in reserves of crude oil. This results in a/an **[f]** _____ in price which would reduce demand.

Something to think about:
Does this cycle/feedback loop have the potential to spiral out of control or does it balance

Laundry detergents remove oil and dirt from clothing. Wastewater from washing clothing enters the sewage system, which will be transported to **[g]** _____. However, if the infrastructure is dysfunctional, high concentrations of LAS can escape into **[h]** _____ which can contaminate water and food and potentially worsen our health. The COVID-19 virus can be removed from clothing with the presence of LAS in laundry detergents, which will better hygiene and **[i]** _____ our health. LAS is cytotoxic at low concentrations causing eczema **[j]** _____ our health. It was reported in a study that LAS at even lower concentrations, when it is no longer cytotoxic, can increase the growth rate of **[k]** _____ cells, which can **[j]** _____ our health.

Something to think about:
Who's health is likely to be more negatively impacted by LAS, and who is likely to be more positively impacted by LAS, rich or poor? Where does a chain of events reflect this in the SOCME?

When waste water treatment plants are dysfunctional, they release raw sewage containing bacteria and viruses directly into river systems. When these facilities are functional, they **[l]** _____ biodegradation of LAS from waste water. Foaming in rivers **[m]** _____ biodegradation. Hence foaming results in **[n]** _____ LAS concentrations for longer increasing the duration of its ecotoxicity.

Question 2 (4 marks)

i. Linear alkylbenzene sulfonate can undergo biodegradation in aerobic conditions to form small organic and inorganic compounds that can be absorbed by bacteria and viruses. **Highlight the arrow** within the biodegradation cycle where the process of biodegradation is considered to be complete. **(1)**

ii. Biodegradation of LAS requires aerobic conditions. How does foaming impact photosynthesis and why does this impact biodegradation rates? Consider the chemical equation for photosynthesis in your answer. **(2)**

Photosynthesis $6\ CO_2 + 6\ H_2O \xrightarrow{\text{light}} C_6H_{12}O_6 + 6\ O_2$

_____

_____

_____

iii. Predict what would happen to the pH of the river if foaming persisted? _____**(1)**

Question 3 (3 marks)

- Complete the given SOCME by filling in **[a]** to **[n]**.
- Draw boundaries around the three main subsystems: economic, environmental and societal.
- Draw boundaries around any additional subsystem groupings.

Question 4 (3 marks)

Discuss these dilemmas, weigh up the risks and benefits and circle a group answer for each.

Fractional distillation vs. global warming
South Africa produces the majority of its energy from burning coal, a fossil fuel, in coal-fired power stations. High temperatures in fractional distillation require more energy which results in increased burning of fossil fuels. This emits more carbon dioxide into the atmosphere and can contribute to global warming and ocean acidification. Laundry detergents are essential, not only during the Covid-19 pandemic but also for keeping good hygiene and clean clothing for everyday use. The kerosene that is used in the production of LAS for laundry detergents, is not burned, but energy is required for its production. As a group we, therefore, think that the societal gain (outweighs / does not outweigh) the environmental consequences.

Sulfonation vs. acid rain/spills
Sulfonation uses sulfur trioxide and sulfuric acid which could lead to acid rain and acid spills into groundwater. This would cause death of aquatic systems and deteriorate the environment. Together with this, laboratory workers can get exposed to strong acids, which contributes to a societal impact with regard to health. Nevertheless, the sulfonation process is required for the production of LAS which has many benefits to society. Therefore, our group thinks that the economic gain (outweighs / does not outweigh) the environmental consequences.

Good quality LABSA vs. Heavy metals
Modified Platinum catalysts are used to obtain a high yield of linear olefins, used for the manufacturing of LAS. It also reduces the production of unwanted branched isomers, produces high quality LABSA and better-performing detergents. With this being said the use of heavy metals during the dehydrogenation reaction can contribute to toxic waste and environmental and societal damage. As a group we have decided that the economic gain (outweighs / does not outweigh) the environmental consequences.

INSTRUCTIONS FOR PRACTICAL ACTIVITY 2 – CONSTRUCTION OF OWN SOCMEs

Use your groups combined subsystem knowledge to create your own SOCME. You may (i) use the given SOCME as a starting point, cutting and pasting sections onto the blank A3 sheet of paper and continuing to add your own ideas or you may (ii) start from scratch with your own ideas.
You will be evaluated on your demonstration of Systems Thinking skills according to the rubric

Sophistication of SOCME	**Low**	**Medium**	**High**	**Dynamic**	Marks
Structure – Concepts added	Adds only one new concept per subsystem with subsystem boundaries	Adds 2 or 3 new independent concepts per subsystem with subsystem boundaries	Adds more than 3 new independent concepts per subsystem with subsystem boundaries		30
Relationships – Linking words (linking words indicate increase/decrease with time if applicable)	Connections drawn between concepts *within* subsystems make the relationship clear	In addition: Connections are drawn between concepts to *link different subsystems* in a sensible relationship	In addition: A few connections are drawn between concepts and *variables* (that can change with time).	In addition: Connections are drawn between *variables* (that can change with time) causing a situation to balance or spiral out of control.	40
Extended application Scenario A or B	Organizes the scenario within and between the existing subsystems and creates new subsystems if necessary to tell the story. (10)		Future predictions are made that show a clear connection and relevance to LAS. (5)		15
				Total	**85**

The extended application component needs you to be able to make predictions. Choose one of the following two scenarios (A or B) to make predictions and show these on your SOCME.

Prediction A
In South Africa, coal-fired power stations depend on fossil fuels for the generation of electricity. SASOL uses the electricity for the fractional distillation to obtain the kerosene used in the manufacturing of linear alkylbenzene sulfonate. When coal is burned, carbon dioxide is emitted. The emitted carbon dioxide can be absorbed by aquatic systems, such as oceans. If excessive carbon dioxide is absorbed, ocean acidification can result, which threatens the life of coral reefs. **Predict** how carbon dioxide emitted during the manufacturing of LAS, can contribute to global warming and expand on the impacts of global warming and its contribution to climate change. You can expand on any of the following: changes in global temperatures, the frequency of natural disasters, malaria and typhoid outbreaks, the impacts of ocean acidification and acid rain on terrestrial and aquatic life.

Prediction B
The Balfour village is one example of a rural community that washes its laundry in the river. There are many other rural and urban communities that don't have access to tap water and thus also wash their laundry in the nearby rivers. The river water from these communities can be polluted with high concentrations of LAS and be oxygen-deficient. River water with decreased oxygen content can influence the rate of LAS biodegradation, the health of aquatic organisms as ecotoxicity changes, ecotourism, and the health of other community members. As the inland river water migrates towards the ocean **predict** how rivers with low oxygen and high concentrations of LAS can threaten surface water sources. You can expand on any of the following: changes in LAS concentrations, river health, ecotoxicity, biodegradation, ecotourism, human health, water-borne diseases, and biodiversity loss.
Include your **Surnames, initials, student numbers, subsystem contributions and Prediction A/B** on the top corner, left-hand side of your SOCME.

An Incomplete Partial SOCME (Quiz 2)