ChemSelect: Example Flame Retardants

Documentation of a case study by Balticfloc

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1 Introduction

ChemSelect is an online application that enables formulators and end users of chemicals to assess the sustainability of substances and mixtures. During its development, ChemSelect was tested by various people on many substances and mixtures. This also included comparisons between two products or more that are intended for the same use and differ in their composition. Some of these couples have been selected as examples. They are used in information materials about ChemSelect and also as training material. We use these reports to describe the examples. In these examples, the experiences gained during evaluating the example chemicals are also documented.

To understand the colour scheme: For each criterion, a colour and a number are assigned that indicate the degree of sustainability: Red/5 not sustainable; Green/1 = sustainable and yellow/3 = "in the middle". If information is missing, the rating is pink/4. If no entry has been made for a criterion, it is grey/-1. If a criterion is not relevant for a substance or use (e.g. persistent for inorganic substances), a light blue/-2 is assigned. Details on the sustainability indicators and the methodology for aggregating the sub-criteria into the main criteria can be found in the evaluation concept.

2 Background information about the products

2.1 Application area and functionality

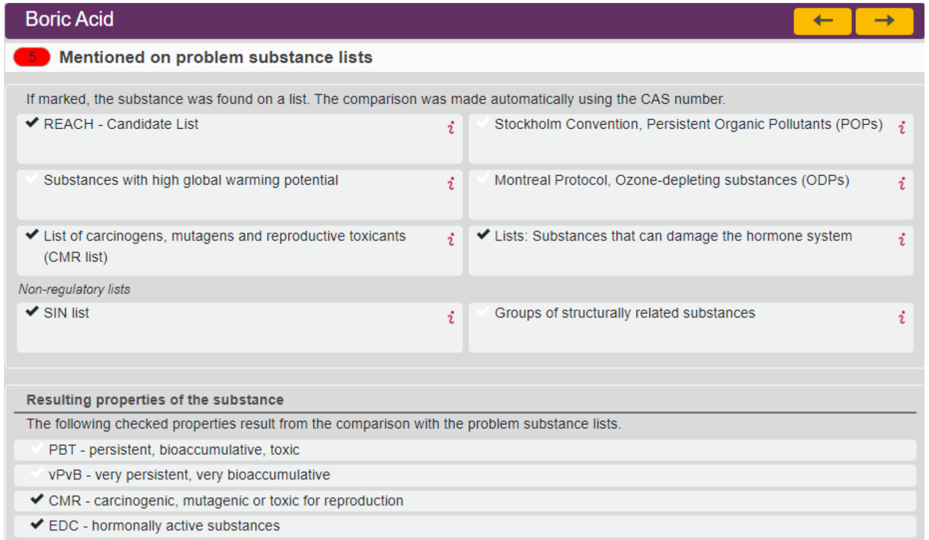
The evaluated products are flame retardants for use in cellulose insulation materials. The flame retardants are mixed with cellulose (paper strips) at Baltifloc, the company conducting the sustainability assessment. The so-treated insulation material is introduced into the buildings by professional users, i.e. construction companies. During service life, the materials are enclosed, and no direct contact of consumers (inhabitants of the house) is possible. The insulation materials (with the flame retardants) are disposed of, when the building is demolished or renovated. Up to now, no specific recovery and recycling of these insulation materials is assumed to exist.

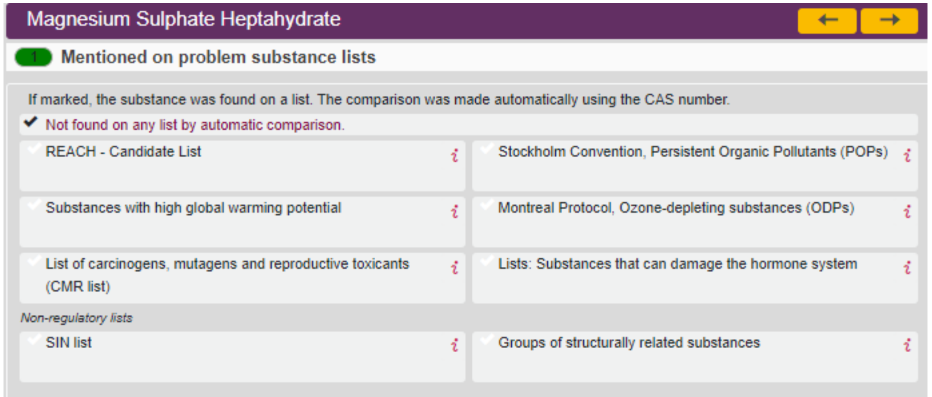
2.2 Details about the compared flame retardants products

Baltifloc aims to phase out the use of Boric Acid, the currently used flame retardant. Two alternatives are assessed: Magnesium Sulphate Heptahydrate and a mixture of Potassium Carbonate and Quartz. In the following, only the comparison of Magnesium Sulphate Heptahydrate with Boric Acid is shown to keep this illustration simple. In the sustainability comparison (c.f. Chapter 4), the mixture is included for a comprehensive overview, too.

3 Assessment

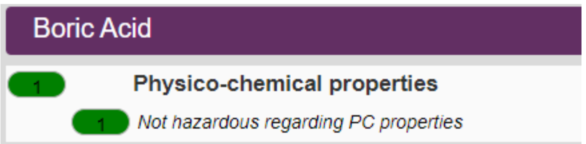
3.1 Lists of problematic substances

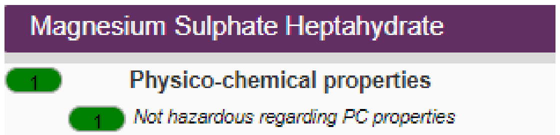




Boric acid is included in the REACH candidate list and listed as potential EDC. This is the reason for Baltifloc to phase out its use. The Magnesium Sulphate Heptahydrate is not included in any list of problematic substances

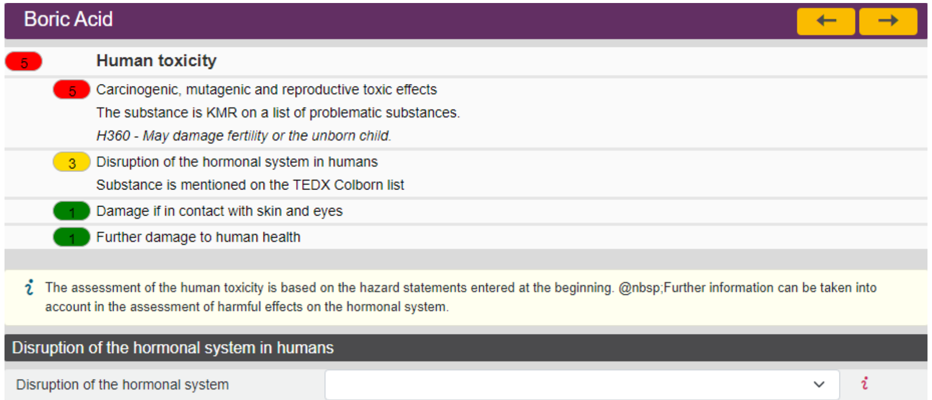
3.2 Physical-chemical properties

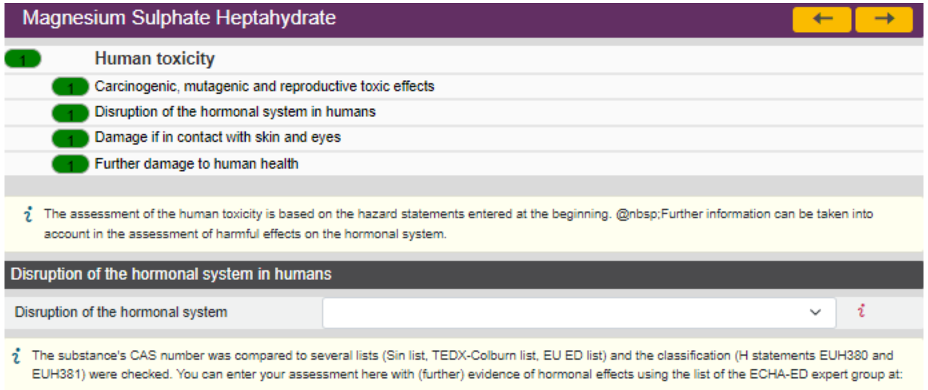




Neither of the two substances has got hazardous physical chemical properties.

3.3 Human toxicity





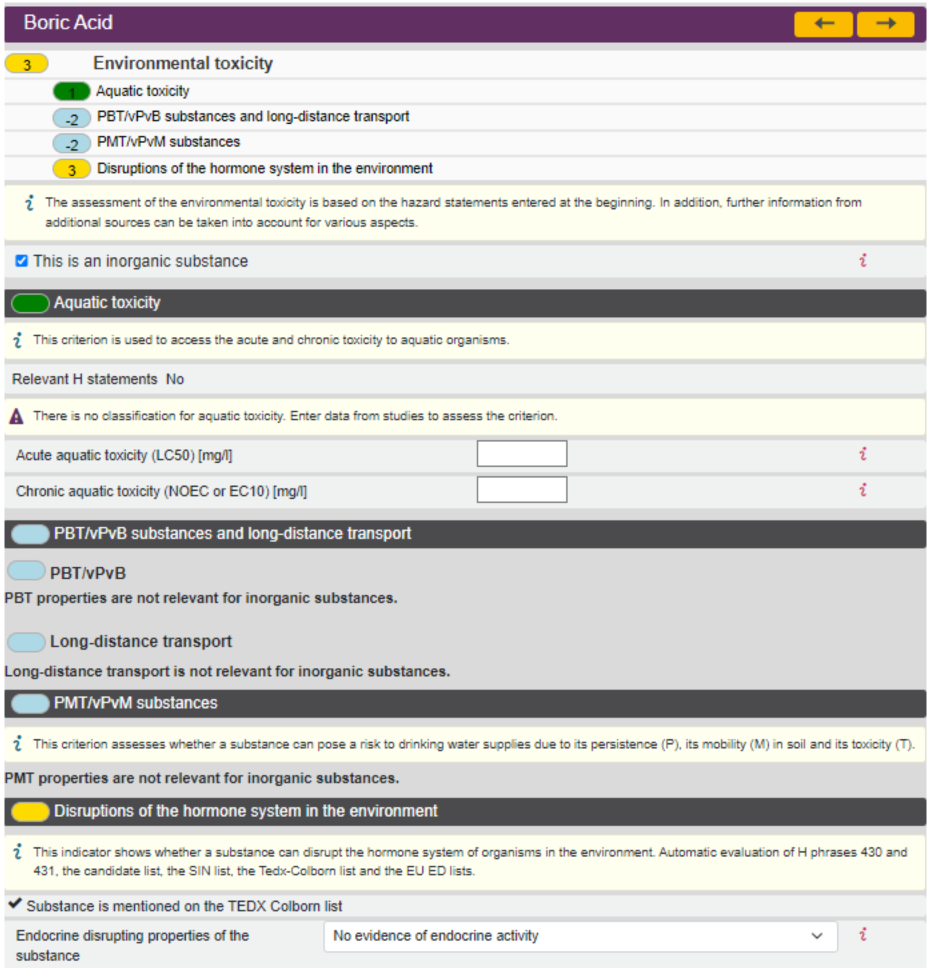
As already evident from the criterion "List of problematic substances", Boric acid is evaluated as red due to its reproductive toxicity and yellow due to its inclusion on a list of substances with suspected or known ED properties. The alternative, magnesium Sulphate Heptahydrate has no classification for human health. Baltifloc also did not find any indications of it being endocrine disrupting.

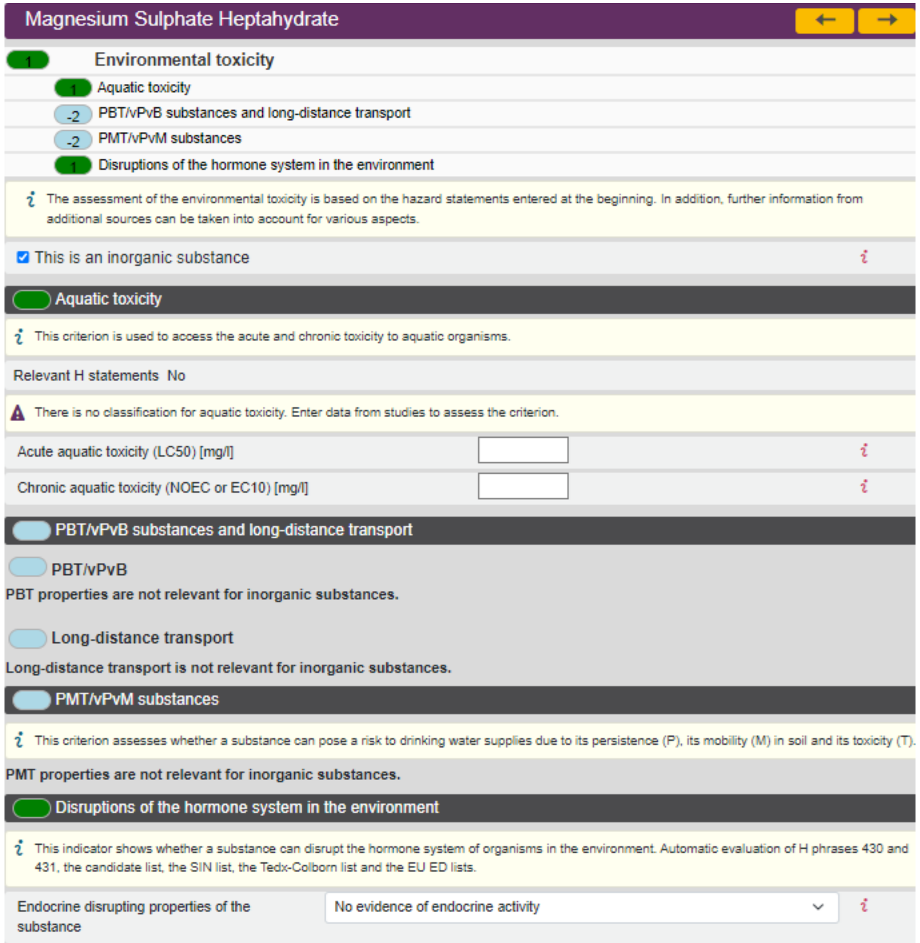
3.4 Environmental toxicity

In the evaluation of the environmental toxicity the criteria PBT/vPvB and PMT/vPvM are not relevant, because both substances are inorganic. In chemicals risk assessment, of inorganic substances, persistence is not addressed as it is the inherent nature of elements and minerals to persist. Hence, the criteria are bright blue for both substances and not considered in the further assessment. Likewise, long range transport is not evaluated for inorganic substances, either.

Both substances are not toxic to the aquatic environment.

Due to the listing in the TEDX Colborn list, boric acid is evaluated yellow with regard to the endocrine disruption in the environment. As it is not a regulatory but an indicative list, the evaluation is yellow and not red. The list entry cannot be overwritten by the fact that there was no evidence of endocrine disruption found in the literature.





Baltifloc entered for Boric acid that they do not have any evidence of endocrine activity. However, as the substance is listed, this does not overwrite the yellow evaluation based on the listing.

3.5 Exposure potential

Boric Acid

1 Exposure potential for workers
1 Exposure potential for consumers
1 Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Scenario | Application quantities | Parameter | Evaluation

Results

Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	0	32	33	7	33
Worker / Inhalative	0	53	33	1	5
Consumer / Dermal		0		2	
Consumer / Inhalative		0		0	
Consumer / Orally		0		2	
Environment / Water	0	40	27	13	40
Environment / Air	0	2	2	4	6
Environment / Soil	0	2	6	4	6

Magnesium Sulphate Heptahydrate

3 Exposure potential for workers
1 Exposure potential for consumers
1 Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Scenario | Application quantities | Parameter | Evaluation

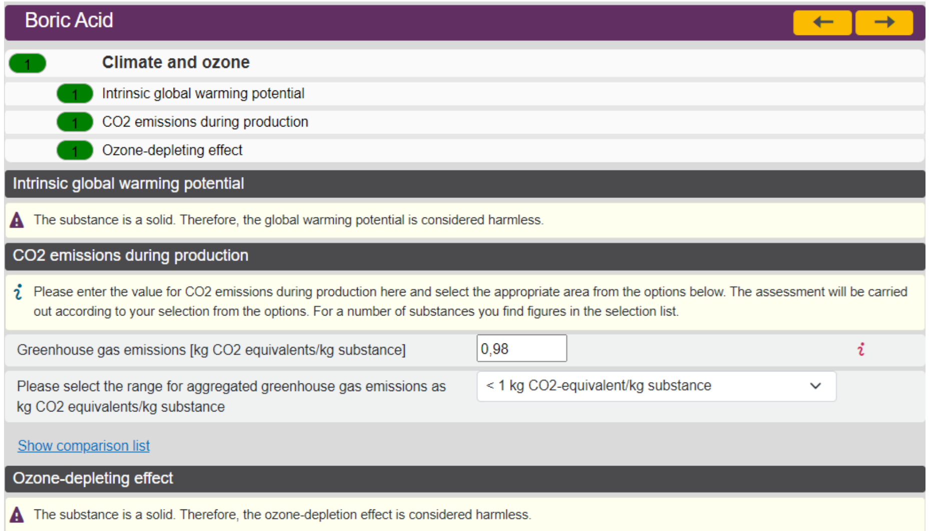
Results

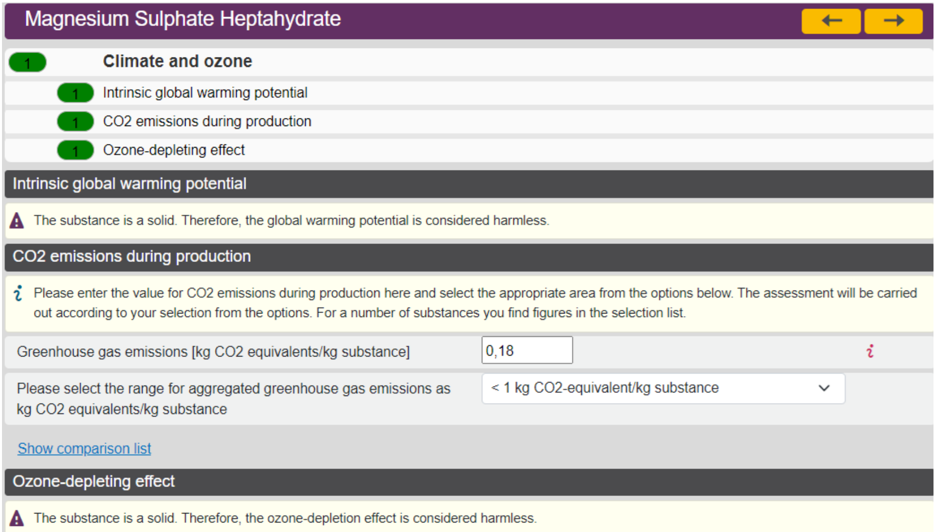
Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	0	48	67	13	67
Worker / Inhalative	0	80	67	2	10
Consumer / Dermal		0		4	
Consumer / Inhalative		0		1	
Consumer / Orally		0		4	
Environment / Water	0	40	27	13	40
Environment / Air	0	2	2	4	6
Environment / Soil	0	2	6	4	6

Both substances are applied in the same “use scenario”. They are mixed with the main insulation materials (“Application”), included in the houses (“Processing Product”), remain in the houses (“use product”) and become waste at the end of the service-life. Hence, the way of application does not differ. The main difference between the two are the uses concentrations, where Magnesium Sulphate Heptahydrate in the ready-to-use insulation material is higher. This leads to higher exposure potentials for workers via dermal and inhalation exposure during the production of the insulation material as well as its introduction into the housing and the waste treatment stage. Therefore, it is evaluated red in some instances, where it is only yellow for the boric acid.

Please note that the concentration ranges are fixed. Magnesium Sulphate Heptahydrate “just” crossed the border to the higher category in the evaluation; the actual difference is not so large. Hence, as the evaluation only allows discrete steps, the difference in exposure potential appears greater than it actually is.

3.6 Climate and ozone impacts



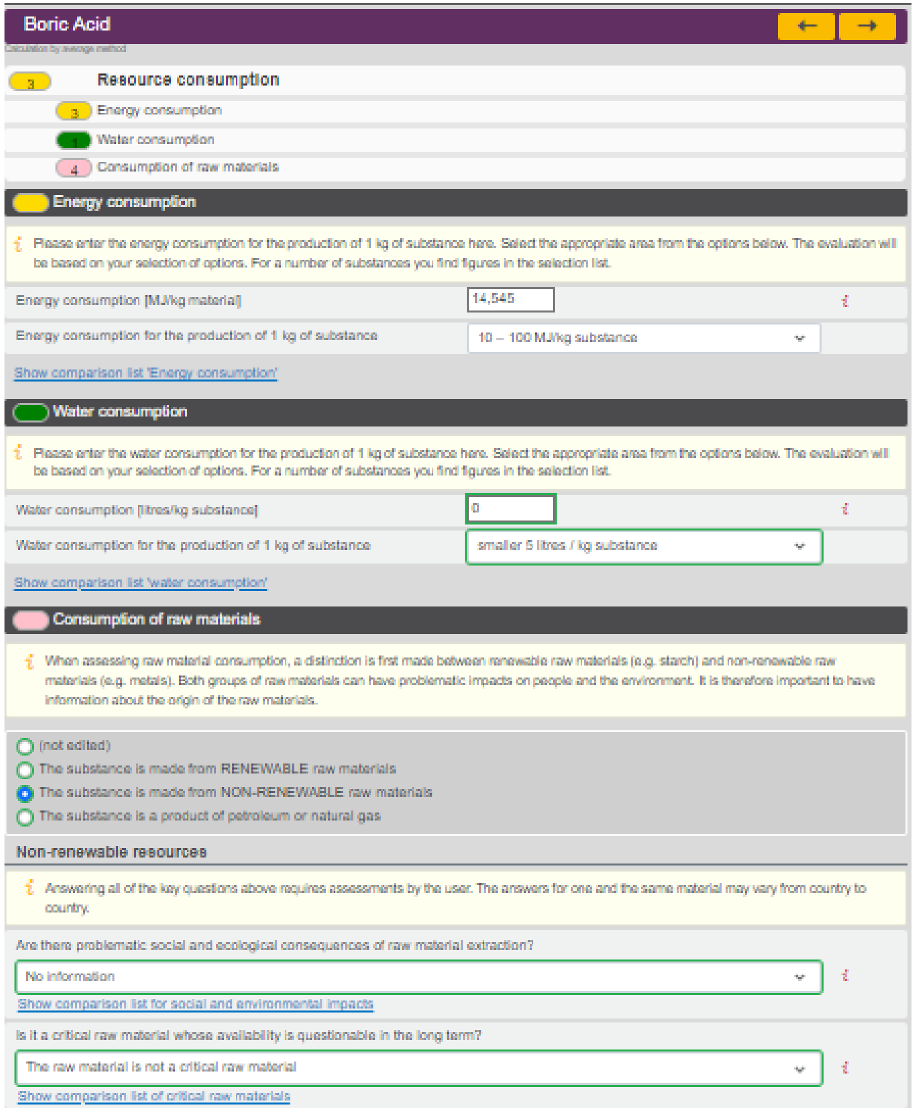


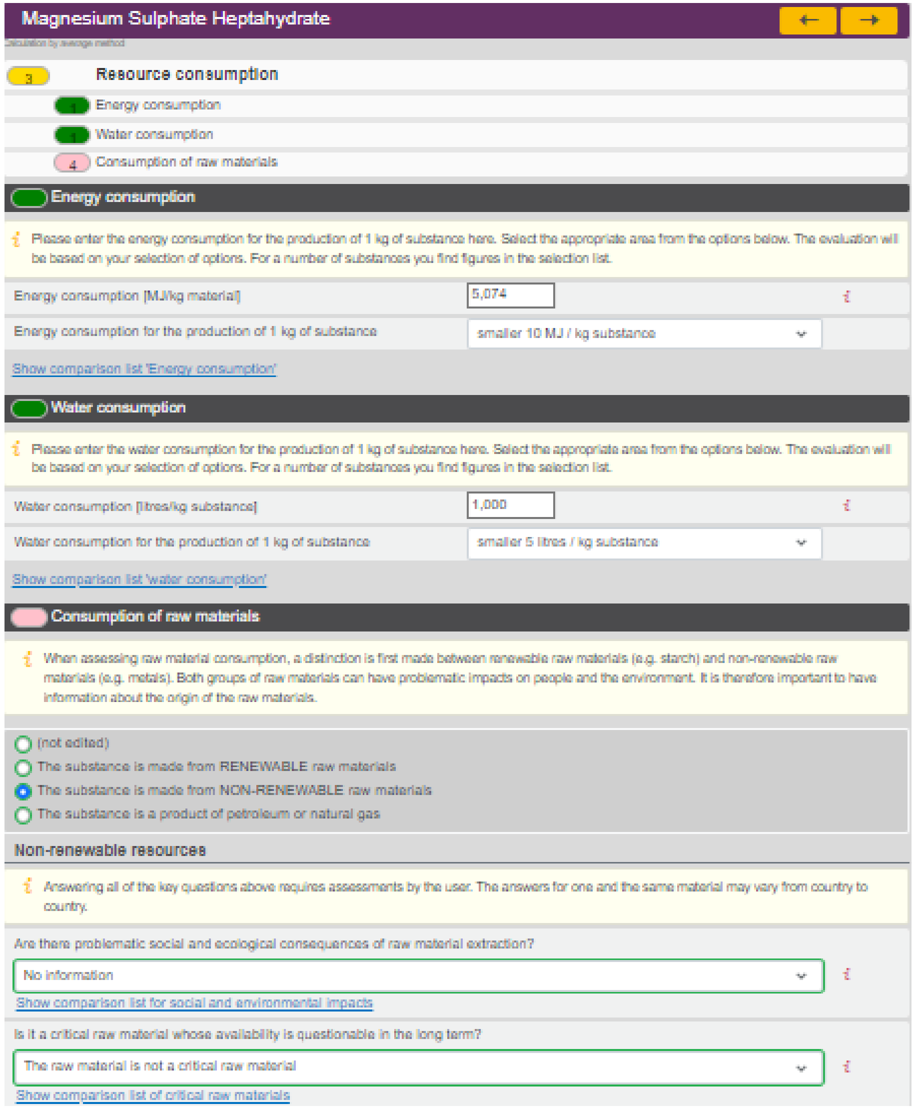
Both substances are inorganic and not very complex. Their exploration is rather "low effort", i.e. the CO2 emissions during their production are relatively low. As both substances are solids, they are evaluated as green regarding their intrinsic greenhouse gas potential and their potential to deplete the ozone layer.

3.7 Resource consumption

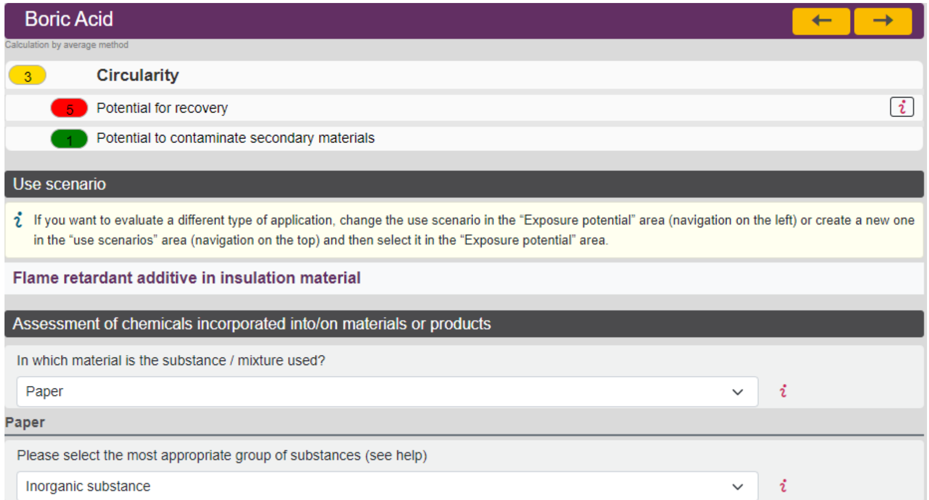
For both substances (or very similar substances) Life Cycle Assessments are available, indicating the energy and water consumption during production. The values are included in ChemSelect and the relating ranges are selected from the picklist.

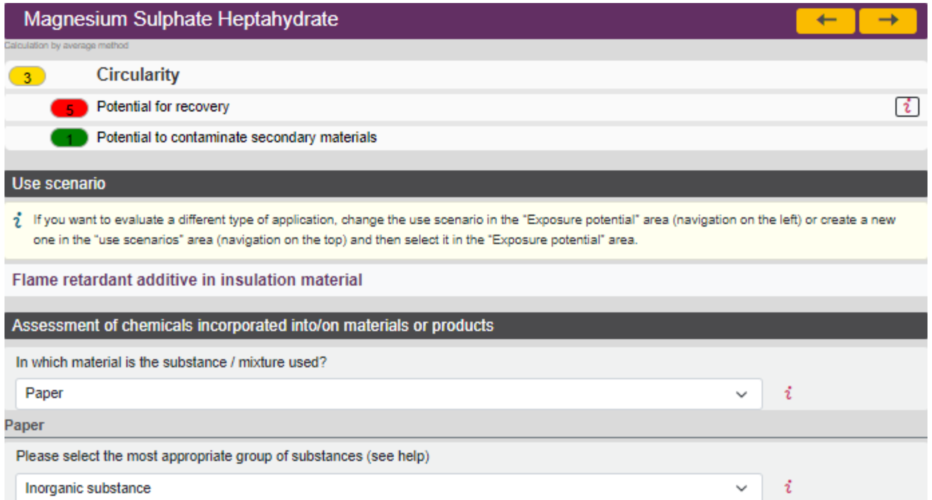
It is unknown whether the extraction of minerals and ores as well as the refinement to obtain the two substances is related to problematic social or ecological consequences. Therefore, the question about raw material consumption is partly answered with "no information", yielding a pink evaluation for this sub-criterion.


Boric Acid
Calculation by average method
3 Resource consumption
3 Energy consumption
1 Water consumption
4 Consumption of raw materials
Energy consumption
Please enter the energy consumption for the production of 1 kg of substance here. Select the appropriate area from the options below. The evaluation will be based on your selection of options. For a number of substances you find figures in the selection list.
Energy consumption [MJ/kg material]
14,545
Energy consumption for the production of 1 kg of substance
10 – 100 MJ/kg substance
Show comparison list 'Energy consumption'
Water consumption
Please enter the water consumption for the production of 1 kg of substance here. Select the appropriate area from the options below. The evaluation will be based on your selection of options. For a number of substances you find figures in the selection list.
Water consumption [litres/kg substance]
0
Water consumption for the production of 1 kg of substance
smaller 5 litres / kg substance
Show comparison list 'water consumption'
Consumption of raw materials
When assessing raw material consumption, a distinction is first made between renewable raw materials (e.g. starch) and non-renewable raw materials (e.g. metals). Both groups of raw materials can have problematic impacts on people and the environment. It is therefore important to have information about the origin of the raw materials.
(not edited)
The substance is made from RENEWABLE raw materials
The substance is made from NON-RENEWABLE raw materials
The substance is a product of petroleum or natural gas
Non-renewable resources
Answering all of the key questions above requires assessments by the user. The answers for one and the same material may vary from country to country.
Are there problematic social and ecological consequences of raw material extraction?
No information
Show comparison list for social and environmental impacts
Is it a critical raw material whose availability is questionable in the long term?
The raw material is not a critical raw material
Show comparison list of critical raw materials


Magnesium Sulphate Heptahydrate
Calculation by average method
3 Resource consumption
1 Energy consumption
1 Water consumption
4 Consumption of raw materials
Energy consumption
Please enter the energy consumption for the production of 1 kg of substance here. Select the appropriate area from the options below. The evaluation will be based on your selection of options. For a number of substances you find figures in the selection list.
Energy consumption [MJ/kg material]
5,074
Energy consumption for the production of 1 kg of substance
smaller 10 MJ / kg substance
Show comparison list 'Energy consumption'
Water consumption
Please enter the water consumption for the production of 1 kg of substance here. Select the appropriate area from the options below. The evaluation will be based on your selection of options. For a number of substances you find figures in the selection list.
Water consumption [litres/kg substance]
1,000
Water consumption for the production of 1 kg of substance
smaller 5 litres / kg substance
Show comparison list 'water consumption'
Consumption of raw materials
When assessing raw material consumption, a distinction is first made between renewable raw materials (e.g. starch) and non-renewable raw materials (e.g. metals). Both groups of raw materials can have problematic impacts on people and the environment. It is therefore important to have information about the origin of the raw materials.
(not edited)
The substance is made from RENEWABLE raw materials
The substance is made from NON-RENEWABLE raw materials
The substance is a product of petroleum or natural gas
Non-renewable resources
Answering all of the key questions above requires assessments by the user. The answers for one and the same material may vary from country to country.
Are there problematic social and ecological consequences of raw material extraction?
No information
Show comparison list for social and environmental impacts
Is it a critical raw material whose availability is questionable in the long term?
The raw material is not a critical raw material
Show comparison list of critical raw materials

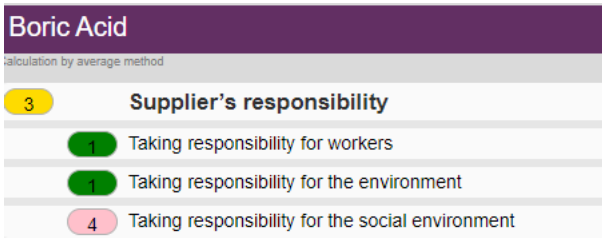
3.8 Circularity potential

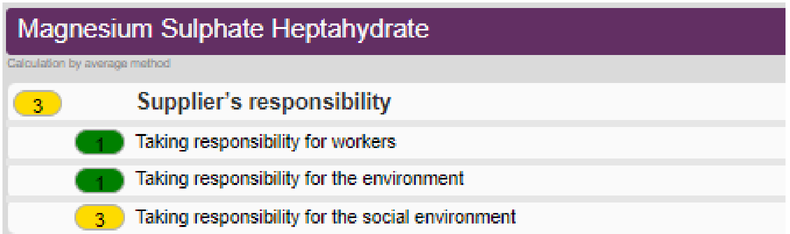




The circularity potential is the same for both substances as they are applied in the same manner.

3.9 Supplier responsibility





Information about the social responsibility of the supplier of boric acid is missing (pink), while of the magnesium sulphate heptahydrate supplier it is known that his social responsibility is medium (yellow).

3.10 Summary

Boric Acid

Aggregated presentation of substance evaluation

If criteria have not yet been worked on (colour grey), they are either evaluated as "realistic worst case - information need!" (colour pink) in this summary or you are asked to work on the criterion in order to enable the evaluation.

5 **Aspect: Particular concern**

Mentioned on problem substance lists

Aspect: Indication of risks for health and environment

An exposure scenario for this substance is available.

5	Workplace	*The substance has properties that are of particular concern. Even if only low levels of exposure are to be expected over the lifetime of the substance, the high level of concern means that there is a high risk potential.*
5	Consumer	*The substance has properties that are of particular concern. Even if only low levels of exposure are to be expected over the lifetime of the substance, the high level of concern means that there is a high risk potential.*
1	Environment	*The substance is rated "yellow" for at least one hazard category. No high levels of exposure occur during the life cycle. This results in a low risk potential.*

3 **Aspect: Life cycle impacts**

Consideration of climate and ozone depletion, resource consumption and circularity.

Magnesium sulphate heptahydrate

Aggregated presentation of substance evaluation

If criteria have not yet been worked on (colour grey), they are either evaluated as "realistic worst case - information need!" (colour pink) in this summary or you are asked to work on the criterion in order to enable the evaluation.

1 **Aspect: Particular concern**

Mentioned on problem substance lists

Aspect: Indication of risks for health and environment

An exposure scenario for this substance is available.

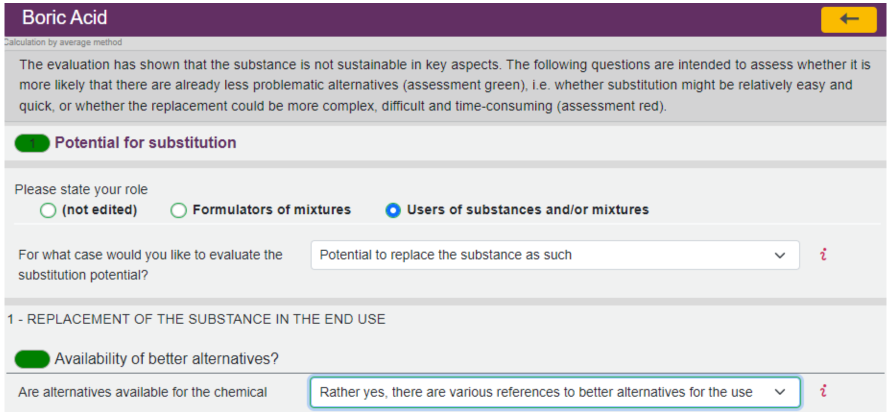
1	Workplace	*According to current knowledge, the substance is not considered dangerous. During the life cycle, at least one situation occurs in which medium exposure is to be expected. Due to the lack of toxicity, the risk potential is low.*
1	Consumer	*According to current knowledge, the substance is not considered dangerous. No relevant exposure is to be expected during the life cycle. Therefore, the risk potential is very low.*
1	Environment	*According to current knowledge, the substance is not considered dangerous. No relevant exposure is to be expected during the life cycle. Therefore, the risk potential is very low.*

3 **Aspect: Life cycle impacts**

Consideration of climate and ozone depletion, resource consumption and circularity.

In the evaluation summary it is evident that the use of magnesium sulphate heptahydrate instead of boric acid is a significant improvement in sustainability. Although the exposure potential was higher for magnesium sulphate heptahydrate due to the absence of known hazards the risk indication results in a green evaluation. For boric acid the risk indication is rated red due to the properties of very high concern for humans.

3.11 Substitution potential



Not needed

The substitution potential of magnesium sulphate heptahydrate is not evaluated as no red result is displayed in the summary. It can be used as a replacement for boric acid and therefore, the assessment of the substitution potential of boric acid is green, i.e. alternatives are available.

4 Sustainability comparison

In the sustainability comparison, two alternatives are compared to the boric acid. The second alternative is a mixture consisting of potassium carbonate and quartz, i.e. a mixture of solid, inorganic substances.

ChemSelect allows comparing substances with substances and mixtures with mixtures. A comparison of a substances with a mixture is technically not possible, yet. Therefore, Baltifloc entered boric acid and magnesium sulphate heptahydrate as “100% - mixtures” and could then compare the two alternatives.

Based on the hazardous properties, it is obvious that both alternatives are better than boric acid. The mixture (pureRed) performs slightly worse in human toxicity than magnesium sulphate heptahydrate due to acute effects on eyes and skin, as well as a classification as toxic to organs.

Mixture	Magnesium Sulphate Heptahydrate	Boric Acid	PureRED
Problem substance lists	1 Rank 1	5 Rank 3	5 Rank 2
Phys. chem. properties	1 Rank 1	1 Rank 1	1 Rank 1
Human toxicity	1 Rank 1	5 Rank 2	5 Rank 3
CMR	1 Rank 1	5 Rank 3	5 Rank 2
Endocrine	1 Rank 1	3 Rank 3	1 Rank 2
Skin/Eye	1 Rank 1	1 Rank 1	3 Rank 2
Other damage	1 Rank 1	1 Rank 1	3 Rank 2
Environmental toxicity	1 Rank 1	3 Rank 3	1 Rank 2
Aquatic Tox.	1 Rank 1	1 Rank 1	1 Rank 1
PBT/vPvB + Remote	1 Rank 2	1 Rank 1	1 Rank 3
PMT/vPvM	1 Rank 2	1 Rank 1	1 Rank 3
Endocrine	1 Rank 1	3 Rank 3	1 Rank 2
Exposure potential in workplaces	3 Rank 3	1 Rank 1	3 Rank 2
Dermal	3 Rank 3	1 Rank 1	3 Rank 2
inhalation	3 Rank 3	1 Rank 1	1 Rank 2
Exposure potential consumers	1 Rank 2	1 Rank 1	1 Rank 2
Dermal	1 Rank 2	1 Rank 1	1 Rank 2
inhalation	1 Rank 2	1 Rank 1	1 Rank 2
Orally	1 Rank 2	1 Rank 1	1 Rank 2
Exposure potential environment	1 Rank 2	1 Rank 2	1 Rank 1
Water	1 Rank 2	1 Rank 2	1 Rank 1
Air	1 Rank 1	1 Rank 1	1 Rank 1
Soil	1 Rank 1	1 Rank 1	1 Rank 1
Climate and ozone	1 Rank 1	1 Rank 1	3 Rank 2
Global warming potential	1 Rank 1	1 Rank 1	1 Rank 2
CO2 emissions	1 Rank 1	1 Rank 1	
Ozone depletion	1 Rank 1	1 Rank 1	1 Rank 2
Resource consumption	3 Rank 1	3 Rank 2	
Energy	1 Rank 1	3 Rank 2	
Water	1 Rank 1	1 Rank 1	
Raw materials	4 Rank 1	4 Rank 1	
Circularity	3 Rank 1	3 Rank 1	3 Rank 1
Recovery	5 Rank 2	5 Rank 2	5 Rank 1
Pollution	1 Rank 1	1 Rank 1	1 Rank 2
Supplier's responsibility	3 Rank 1	3 Rank 2	3 Rank 2
Worker	1 Rank 1	1 Rank 1	1 Rank 1
Environment	1 Rank 1	1 Rank 1	1 Rank 1
Social environment	3 Rank 1	4 Rank 2	4 Rank 2

The differences in the exposure potential are due to the different concentrations of the flame retardants in the final insulation material as well as differences in water solubility.

The PureRed mixture lacks information about lifecycle impacts, while this is available for the other two chemicals. No ranks are assigned to criteria which have not been assessed (grey).

As information on "climate and ozone" has been entered (due to all being inorganic solids, both GWP and ODP are green), here the colour is pink. For resource consumption, no information is entered, therefore, the criterion is not included in the assessment.

5 Conclusions

The evaluation clearly shows that both alternatives are better than the use of boric acid. The magnesium sulphate heptahydrate is the best option also with regard to the level of certainty about lifecycle impacts. As a next step, the further information could be sought for the life cycle impacts and/or the exposure situations could be further assessed. However, as both options appear to be possible, it is advisable to test both alternatives in practice, in order to also include performance information in the final decision making.