ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 8 December 2017

Addressee: [redacted]

Decision number: CCH-D-2114382055-51-01/F
Substance name: 39947_Reaction mass of 1-(3-((C12-18-(even numbered))-alkyl-amino)propyl)guanidine acetate salt and 1-(C12-18-(even numbered))-alkyl-1-(3-guanidinopropyl)guanidine acetate salt and 1-(C12-18-(even numbered))-alkyl-tetrahydropyrimidin-2(1H)-imine acetate salt
EC number: 939-650-3
CAS number: NS
Registration number: [redacted]
Submission number: [redacted]
Submission date: 30.09.2016
Registered tonnage band: 100-1000T

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the REACH Regulation), ECHA requests you to submit information on:

1. **Name or other identifier of the substance (Annex VI, Section 2.1.);**
   - **Manufacturing process**
2. **Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.; test method: Aerobic mineralisation in surface water – simulation biodegradation test, EU C.25./OECD TG 309) at a temperature of 12 °C with the registered substance;**
3. **Soil simulation testing (Annex IX, Section 9.2.1.3.; test method: Aerobic and anaerobic transformation in soil, EU C.23./OECD TG 307) at a temperature of 12 °C with the registered substance;**
4. **Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24./OECD TG 308) at a temperature of 12 °C with the registered substance;**
5. **Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: OECD TG 305-III: Dietary Exposure Bioaccumulation Fish Test) with the registered substance;**

You may adapt the testing requested above according to the specific rules outlined in Annexes VI to X and/or according to the general rules contained in Annex XI to the REACH Regulation. To ensure compliance with the respective information requirement, any such adaptation will need to have a scientific justification, referring and conforming to the appropriate rules in the respective annex, and adequate and reliable documentation.

You have to submit the requested information in an updated registration dossier by **15 December 2020**. You also have to update the chemical safety report, where relevant. The timeline has been set to allow for sequential testing.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2 and advice and further observations are provided in Appendix 3.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

Authorised[1] by Kevin Pollard, Head of Unit, Evaluation E1

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

Appendix 1: Reasons

1. Name or other identifier of the substance (Annex VI, Section 2.1.)

In accordance with Article 10(a)(ii) of the REACH Regulation, the technical dossier must contain information on the identity of the substance as specified in Annex VI, Section 2 to the REACH Regulation. In accordance with Annex VI, Section 2 the information provided has to be sufficient to enable the identification of the registered substance.

Annex VI, section 2.1 of the REACH Regulation requires that the registration dossier contains adequate and sufficient information to enable each substance to be identified. According to chapters 4.2 and 4.3 of the "Guidance for identification and naming of substances under REACH and CLP" (version 2.1, May 2017) – referred to as "the SID Guidance" thereinafter, the following applies:

a) a multi-constituent substance is a substance defined by its composition, for which more than one main constituent is present at a concentration ≥ 10% (w/w) and < 80% (w/w). A multi-constituent substance should be named as a reaction mass of the main constituents of the substance.
b) a substance as of Unknown or Variable composition, Complex reaction products or Biological materials, also called UVCB substance, is a substance that cannot be sufficiently identified by the chemical composition, because for example the number of constituents is relatively large and/or the composition is, to a significant part, unknown and/or the variability of composition is relatively large or poorly predictable. The naming of a UVCB substance should consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process.

In the current dossier, you have identified the substance as a multi-constituent substance, with the IUPAC name: [redacted]. The following remark was given: "*Molecular formular, SMILES notation and molecular weight range cannot be given as substance is a reaction mass.*" The description of the manufacturing process was not provided, instead the following was reported: "*Manufactured by Toll manufacturer.*"

In IUCLID section 1.2, you reported under "Constituents" three groups of constituents, each of them consisting of several [redacted] For each group of constituents you provided in the description field the following information concerning the identity of the "[redacted]" term: "[redacted]". In IUCLID section 1.4, the analytical report on page 4 and page 13 contains the following C-chain length distribution: [redacted].

Based on the information contained in sections 1.2 and 1.4 of the IUCLID dossier, due to the large number of constituents (*i.e.* each group of constituents contains up to 7 components), the substance should be regarded as a UVCB substance, rather than a well-defined multi-constituent substance. Thus the identification should be done according to chapter 4.3 of the SID guidance, rather than to chapter 4.2, which means that a description of the manufacturing process should be provided. In addition, the carbon chain length

composition appears to be not fully consistent in IUCLID sections 1.2 and 1.4. In particular, [redacted] is reported with a minimum concentration range of [redacted]% in section 1.2, but in section 1.4 it is reported with a detected area % of [redacted] which is outside the range reported in section 1.2.

Consequently, you need to provide additional information to verify the identity of the substance as follows:

In IUCLID 1.1 you should select the appropriate substance type, i.e. UVCB.

In IUCLID 1.2 you should provide a detailed description of the manufacturing process. In particular the identity of the starting materials used for manufacturing the substance (including the chain length distribution which should be in line with the analytical data reported in IUCLID section 1.4 for the final product). Also, the relevant steps and process parameters (*e.g.* temperature, pressure) that affect the composition and therefore the identity of the substance. You should note that based on the OECD No. 193 (OECD Guidance for Characterising Oleochemical Substances for Assessment Purposes)[2] for a composition-based characterisation, all alkyl chains, whose concentration is above 10% (based on the maximum concentration value of the concentration range), should be part of the characterisation (i.e. included in the name). Therefore, it is important that the carbon chain length distribution (including the ranges) is representative of the registered substance, is clearly reported and in line with the analytical data.

The manufacturing process description of the substance shall be included in the "Description of the composition" field in IUCLID section 1.2. In addition, by selecting the UVCB substance type, you should report your composition without differentiating between main constituents and impurities, but all components as constituents (and/or groups of constituents). The carbon chain length distribution shall be provided in the composition description, in section 1.2. In case the updated carbon chain distribution is not anymore in line with the chemical name provided in section 1.1, the chemical name must be revised accordingly, following the recommendations provided by the OECD Guidance for Characterising Oleochemical Substances for Assessment Purposes.

Further technical details on how to report the composition of UVCB substances in IUCLID are available in the ECHA Guidance on how to report the identity of the substance (SID Guidance).

2., 3. & 4. Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.), Soil simulation testing (Annex IX, Section 9.2.1.3.), Sediment simulation testing (Annex IX, Section 9.2.1.4.)

In accordance with Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to IX to the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Simulation testing on ultimate degradation in water" is a standard information requirement as laid down in Annex IX, Section 9.2.1.2.of the REACH Regulation. "Soil simulation testing" is a standard information requirement for substances with a high potential for adsorption to soil, as laid down in Annex IX, Section 9.2.1.3. of the REACH Regulation and "sediment

[2] http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)6&doclanguage=en

simulation testing" is a standard information requirement for substances with a high potential for adsorption to sediment, as laid down in Annex IX, Section 9.2.1.4. of the REACH Regulation. ECHA notes that the this substance is deemed to be highly adsorptive, as you explained in your registration dossier. Therefore it has a high potential for adsorption to sediment and to soil and information on soil and sediment is required as well.

Adequate information on these three endpoints needs to be present in the technical dossier for this registered substance to meet these information requirements.

You have sought to adapt the above mentioned information requirements. You provided the following justification for your approach:

"GENERAL REMARKS
Issues in Biodegradation testing of the registration substance
The registration substance is toxic to microorganisms and therefore the test concentration in biodegradation tests have to be sufficiently low to ensure the viability of the inoculum. This means that ^{14}C test item would be the test material of choice. As the registration substance is a multi-constituent the preparation of a representative ^{14}C material is not feasible. Therefore cold material has to be used which poses a considerable analytical challenge at very low concentration. On the other hand results from similar mono-constituent ^{14}C substances can be reasonably used for read-across.

Read across substances
The registration substance has structural elements like long-chain ammonium and alkyl guanidinium salts. Such structural elements are present in long-chain primary alkyl amines and in guanidinium salts. In the following read-across substances are listed which are all REACH registered and where the substance data can be found on the Dissemination site of ECHA (http://echa.europa.eu/ information-on-chemicals) or at the EU ESIS site (http://esis.jrc.ec.europa.eu):
Gudanidinium nitrate, CAS No, 506 -93 -4
1-Hexadecanamine, CAS No. 143 -27 -1
Cocoylamines (C12 -14 Primary alkyl amines), CAS No. 61788 -46 -3
C20 -22 alkyl trimethyl ammonium chloride, CAS No. 68607-24-9

BIODEGRADATION IN WATER: SCREENING TESTS
The registration substance is toxic to microorganisms and the required minimum test concentration of e.g. 5 mg/L in a test on ready biodegradation is too high to allow conditions which are not influencing the viability of the inoculum. As it is not feasible to prepare ^{14}C material of the registration substance (see above) a test at lower concentration could not be performed. Instead read-across is used to justify the conclusion that the registration substance is readily biodegradable:
^{14}C-C22 alkyl trimethyl ammonium chloride (see IUCLID Chapter 5.2.1):
OECD 301 B CO_2 Evolution test, 0.2 mg/L test conc.: 80% $^{14}CO_2$ formation after 28d
C12 -14 alkyl amines (see IUCLID Chapter 5.2.1):
OECD 301B CO_2 Evolution test, 13 mg/L test conc. : >60% CO_2 formation after 29d, readily biodegradable
Guanidinium nitrate (see ESIS web, CAS 506 -93 -4)
^{14}C Guanidinium nitrate (no concentration given) was incubated with industrial sewage as inoculum and showed 68% $^{14}CO_2$ formation after 1.3 days.
CONCLUSION
Based on the available facts (see above), it can be concluded that the registration substance is likely to be readily biodegrable if the concentration of the registration substance is low enough to ensure the viability of the inoculum.

BIODEGRADATION IN WATER & SEDIMENT
SEWAGE TREATMENT PLANT SIMULATION TEST
An OECD 303A STP Simulation test is carried out with cold registration substance. This is a considerable analytical challenge as low test concentration is warranted due to the high toxicity for microoganisms. For the time being read-across is used (see IUCLID Chapter 5.2.2):
C20 -22 alkyl trimethyl ammonium chloride (see IUCLID Chapter 5.2.2)
OECD 303 A: Mean elimination: 99%, mean biodegradation: 92.2% (6.9% sorbed to sludge, 1% to effluent)
Cocoylamines (C12 -14 Primary alkyl amines, see IUCLID Chapter 5.2.2)
OECD 303A: Mean elimination: 99.8%, mean biodegradation: not measured

SIMULATION TEST ON BIODEGRADATION IN SEDIMENT
It is reasonable to use the DT50 of the soil biodegradation simulation test for sediment as well (see REACH Guidance) and therefore no OECD 308 Sediment simulation test is warranted.
OECD 307: highest DT50 soil is 45.5 d at 12 deg C

CONCLUSION
STP
The results from the OECD303A with C20 -22 ATQ is used as worst case for the registration substance resulting in 92.% biodegradation, 6.9% sorption to sewage sludge and 1% discharge in effluent.
SEDIMENT
The DT50 of 45.5 d from an OECD 307 soil study with C20 -22 alkyl trimethyl ammonium chloride is used a worst case for the registration substance.

BIODEGRADATION IN SOIL
For a Soil biodegradation simulation test according OECD 307 ^{14}C material is mandatory to achieve reliable results. As mentioned before the registration substance is a multi-constituent and the synthesis of a representative ^{14}C material not feasible. Therefore read-across is the only way to conclude on soil biodegradation:
^{14}C-C22 alkyl trimethyl ammonium chloride (see IUCLID Chapter 5.2.3)
OECD 307: highest DT50 is 45.5 d at env. temperature 12 deg C is used in exposure assessment of the registration substance
^{14}C-1 -Hexadecanamine (see IUCLDI Chapter 5.2.3)
OECD 307: highest DT50 is 17 d at env. temperature 12 deg C

CONCLUSION
Both read-across substances show rapid degradation in soil. The worst case result from the OECD 307 carried out with ^{14}C-C22 alkyl trimethylammonium chloride which is DT50 45.4 d at 12 deg C is used in exposure assessment of the registration substance".

Although you did not specify the provisions allowing adaptation, ECHA interprets your attempt as a combination of adaptations according (a) Annex XI, Section 1.5 "read-across" and (b) Annex XI, Section 2, "technical feasibility". ECHA considered additionally (c) column 2 adaptation possibilities. ECHA evaluated and concluded on the potential adaptations as the following:

a) Read-across hypothesis (Annex XI, Section 1.5.)

Article 13(1) of the REACH Regulation provides that information on intrinsic properties of substances may be generated by means other than tests, "*provided that the conditions set out in Annex XI are met*". This annex proposes some general rules for adapting the standard information requirements set out in Annexes VII to X of the REACH Regulation.

In particular, Annex XI, Section 1.5. of the REACH Regulation introduces the concept of read-across. This concept is based on the identification of similar compounds. Information for one or more source substances or reference substances may be used to make a prediction for the target substance (i.e. the registered substance). According to Annex XI, Section 1.5., two conditions shall be necessarily fulfilled. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group (read-across approach). Based on the above, a read-across hypothesis needs to be provided. This hypothesis establishes why a prediction for a toxicological or ecotoxicological property is reliable and should be based on recognition of the structural similarities and differences between the source and registered substances[3]. This hypothesis explains why the differences in the chemical structures should not influence the toxicological/ ecotoxicological properties or should do so in a regular pattern.

The read-across approach must be justified scientifically and documented thoroughly, also taking into account the differences in the chemical structures. There may be several lines of supporting evidence used to justify the read-across hypothesis, with the aim of strengthening the case.
You have provided study summaries with the following read-across substances:

- Cocoylamines (C12 -14 Primary alkyl amines) (CAS: 61788-46-3): "*Determination of the removal of cocoamine in a simulation test of an activated sludge plant treating industrial wastewater*" ([redacted], 2002), according to OECD test guideline 303A,

- Quaternary ammonium compounds, C20-22-alkyltrimethyl, chlorides (CAS: 68607-24-9), "*C20/22 ATQ trocken Simulation Test - Aerobic Sewage Treatment acc. to OECD 303 A: Activated Sludge Units*" ([redacted], 2010), according to OECD test guideline 303A,

- Docosyltrimethylammonium chloride (CAS: 17301-53-0), "*[^{14}C]C22-ATQ: Degradation in Three Soils Incubated under Aerobic Conditions*" ([redacted], 2011), according to OECD test guideline 307,

- Hexadecanamine (CAS: 771435-48-4), "*1-Hexadecanamine: Degradation in Three Soils Incubated under Aerobic Conditions*" ([redacted] 2010), according to OECD test guideline 307,

In addition, you have indicated in your chemical safety report (CSR) that another analogue substance Guanidinium nitrate (CAS: 506 -93 -4) was readily biodegradable, but you did not provide a study summary in IUCLID for this substance.

[3] Please see for further information ECHA *Guidance on information requirements and chemical safety assessment* (version 1, May 2008), Chapter R.6: QSARs and grouping of chemicals.

ECHA understands that you make a read-across hypothesis that "*The registration substance has structural elements like long-chain ammonium and alkyl guanidinium salts. Such structural elements are present in long-chain primary alkyl amines and in guanidinium salts.*" You assume that the available information on the properties of the analogue substances, and in particular the fact that none of these substances is likely to persist in the environment, allow prediction that the registered substance is readily biodegradable. However ECHA considers your read-across justification is not adequate to prove so, as explained below.

The registered substance is a cationic surfactant which contains structural elements like long-chain primary alkyl ammonium (hydrophobic tail of the substance) and alkyl guanidinium (hydrophilic (cationic) headgroup of the substance) salts covalently bound together. The information provided in the dossier for the read-across substances suggests that both these long-chain primary alkyl ammonium and alkyl guanidinium salts are biodegradable when considered *separately*. However, your approach has not demonstrated whether they will be biodegraded when covalently bound together. The literature on surfactants indeed suggests that it is the primary degradation, and in particular the cleavage of the bond between the hydrophilic headgroup and the hydrophobic tail, which most heavily impacts the ultimate biodegradability of a surfactant. Your approach has not demonstrated whether the primary degradation of the registered substance will be rapid.

ECHA notes that the registered substance is highly adsorptive and toxic to microorganisms. ECHA considers that the primary degradation of the substance may be hindered by the high potential for adsorption and the toxicity of the substance. Because of its high potential for adsorption, the substance is expected to adsorb to solid particles (i.e. onto suspended matter in water and STP, onto sediment, onto soil). This could limit its bioavailability to degrading microorganisms. Furthermore, the concentration on the surface of the particles may be high enough to exert locally inhibitory toxic effects to the microorganisms.

Therefore, ECHA considers that your read-across hypothesis is inadequate to support your claim that the registered substance is readily biodegradable and to demonstrate that it is not persistent. Therefore your read-across adaptation is rejected.

b) Technical feasibility of the tests (Annex XI, Section 2.)

Annex XI, Section 2. of the REACH Regulation provides some provisions for substances for which testing is technically not possible because of the properties of the substance.

In your justification, you explain that ready biodegradation tests are not feasible at the test concentrations required for those tests (typically from 2 mg/L to 100 mg/L) because the registered substance is toxic to microorganisms (it is used as disinfectant) and those test concentrations are too high to allow conditions which are not influencing the viability of the inoculum.

For simulation tests much lower test concentrations should be used, but you claim that this would pose "*a considerable analytical challenge*". You further claim that using a radiolabelled test item is not possible either because the preparation of a representative ^{14}C material would not be feasible for a multiconstituent or UVCB substance. On this basis, you proposed to apply a read-across approach as explained in section 2(a) above.

ECHA notes that Annex II of OECD test guideline 301 proposes some guidance for testing the biodegradability of substances suspected to be toxic to the inoculum. In particular it is

recommended that the test concentration should be less than 1/10 of the EC50 values (or less than EC20 values) obtained for aquatic microorganisms.

The following values are reported in the registration dossier for the toxicity to aquatic microorganisms (Annex VIII, Section 9.1.4. of the REACH Regulation):

- 3h-EC50: 28.4 mg/L and 3h-NOEC: 10 mg/L from a first study according to OECD test guideline 209 (Noack, 2013),

- 16h-EC50: 23 mg/L and 16h-EC20: 9 mg/L from a second study according to OECD test guideline 209 (Hoechst AG, 1994).

These results suggest that a ready biodegradability test could be technically feasible with the registered substance using test concentrations of not less than 2 mg/L, in accordance with the recommendations of Annex II of OECD test guideline 301.

With regard to the feasibility of radiolabelling, ECHA notes that the guanidinium group is common to every constituent of the registered substance and could be used for radiolabelling. If radiolabelling is technically feasible, then simulation tests can be performed.

Therefore ECHA considers that you have not demonstrated that the ready biodegradability tests or the simulation tests are technically not feasible with the registered substance.

c) Adaptation according to Annex IX, Section 9.2., column 2

Column 2 of Section 9.2. of Annex IX of the REACH Regulation specifies that simulation tests need to be conducted if the chemical safety assessment according to Annex I of the REACH Regulation indicates the need to investigate further the degradation of the substance and its degradation products and that the choice of the appropriate test(s), which may include simulation degradation tests in appropriate media, depends of the results of the chemical safety assessment.

ECHA notes that the lowest value for chronic toxicity to aquatic organisms is a 72h-ErC10 (72h) of 4 µg/L for algae (= 0.004 µg/L). Therefore the substance meets the T criterion of "EC_{10} < 0.01 mg/L" for the PBT assessment as detailed in Annex XIII of the REACH Regulation.

ECHA further notes that no adequate information is available with regard to the potential bioaccumulation of the substance (see section 5 of the present decision). It is therefore not possible to conclude whether the substance meets the B/vB criterion for the PBT/vPvB assessment as detailed in Annex XIII of the REACH Regulation.

ECHA considers that, as your read-across adaptation is rejected as described in subsection (a) above, there is no adequate information available with regard to the potential persistence of the substance. It is therefore not possible to conclude whether the substance meets the P/vP criterion for the PBT/vPvB assessment as detailed in Annex XIII of the REACH Regulation.

Therefore ECHA considers that your chemical safety assessment does not rule out the possibility that your substance could be PBT or vPvB. For the purpose of the PBT/vPvB assessment, the persistence of the substance needs to be investigated for every relevant environmental compartment.

Column 2 of Sections 9.2.1.2. of Annex IX of the REACH Regulation indicates that the simulation testing on ultimate degradation in surface water does not need to be conducted if the substance is highly insoluble in water or if the substance is readily biodegradable.

Column 2 of Section 9.2.1.3. of Annex IX of the REACH Regulation indicates that soil simulation testing does not need to be conducted if the substance is readily biodegradable or if direct and indirect exposure of soil is unlikely.

Column 2 of Section 9.2.1.4. of Annex IX of the REACH Regulation indicates that simulation testing does not need to be conducted if the substance is readily biodegradable or if direct and indirect exposure of sediment is unlikely.
ECHA notes the following points:

- As explained in subsection (a) above, it is not demonstrated that the registered substance is readily biodegradable.

- According to your registration dossier, the water solubility value of the substance (corresponding to the critical micelle concentration) was determined to be about 280 mg/L at 20°C whereas the test concentrations recommended for a simulation test in water are between 1 and 10 µg/L. Furthermore, the available values of toxicity for aquatic microorganisms are well above those values. ECHA concludes that the water solubility of the registered substance as well as the toxicity values for aquatic microorganisms are consistent with the performance of a simulation test in water according to OECD TG 309.

- As you explained in your registration dossier, you consider this registered substance as being highly adsorptive. It has therefore a high potential for adsorption to sediment and to soil. The substance is used as disinfectant with wide-dispersive uses. When released to water, it will tend to adsorb onto suspended matter and sediment. Exposure of sediment is thus likely. The registered substance is expected to be released mainly to sewage treatment plants where it can adsorb to the sludge. This sludge may be applied to agricultural soils and therefore indirect exposure to soil is also likely.

Therefore ECHA considers that the specific rules for adaption of column 2 of Annex IX, Section 9.2.1.2., Section 9.2.1.3. and of Section 9.2.1.4. of the REACH Regulation are not met and an adaptation according column 2 is not possible.

d) Summary of the outcome of sections a-c

As explained above, you have sought to adapt the information requirements for "Simulation testing on ultimate degradation in water", "Soil simulation testing" and "Sediment simulation testing". However ECHA considers, as explained above, that your adaptations neither meet the specific rules for adaptation of column 2 of Annex IX, Section 9.2 of the REACH Regulation, nor the general rules for adaptation of Annex XI of the REACH Regulation. Consequently there are information gaps and it is necessary to provide information for these endpoints.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017):

- Aerobic mineralisation in surface water – simulation biodegradation (test method EU

C.25. / OECD TG 309) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.2.
- Aerobic and anaerobic transformation in soil (test method EU C.23. / OECD TG 307) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.3.
- Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24./OECD TG 308) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.4.

One of the purposes of the simulation tests is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of the REACH Regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "*attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids* [...]*, and a typical temperature that represents the particular environment*". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-9 (version 3.0 February 2016) indicates 12°C (285K) as a plausible representative environmental temperature for the EU to be used in the chemical safety assessment. Therefore, the test results, and in particular the degradation rates and the substance half-life, shall correspond to the temperature of 12°C (285K).

In the OECD TG 309 Guideline two test options, the 'pelagic test' and the 'suspended sediment test', are described. For the 'suspended sediment test', surface sediment is artificially added to the test medium whereas the 'pelagic test' naturally contains suspended matter. ECHA considers that the 'pelagic test' option should be followed as that is the recommended option for the P assessment. The amount of suspended solids in the pelagic test should be representative of the level of suspended solids in EU surface water. The concentration of suspended solids in the surface water sample used should therefore be approximately 15 mg dw/L. Testing natural surface water containing between 10 and 20 mg SPM dw/L is considered acceptable. The formation of NERs may consequently be significant in surface water tests too. Similarly to the tests in sediment and soil, you should thus quantify NERs formed during the test in surface water and explain and scientifically justify the extraction procedure and solvent used.

Furthermore, simulation tests with highly adsorptive substances performed in sediment (OECD TG 308) or in soil (OECD TG 307) possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product. The amount and kind of NERs is operationally defined by the extraction method employed. When reporting the NERs in your test results you are requested to explain and scientifically justify the extraction procedure and solvent used for obtaining a quantitative measure of the NERs.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision:
- Aerobic mineralisation in surface water – simulation biodegradation test (test method: EU C.25./OECD TG 309)
- Aerobic and anaerobic transformation in soil (test method: EU C.23./OECD TG 307).

- Aerobic and anaerobic transformation in aquatic sediment systems (test method: EU C.24./OECD TG 308)

Notes for your consideration

Before conducting the requested tests you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Sections R.7.9. (version 4.0, June 2017) and Chapter R.11, Section R.11.4.1.1 on PBT assessment (version 3.0, June 2017) to determine the sequence in which the simulation tests are to be conducted and the necessity to conduct all of them.

In accordance with Annex I, Section 4, of the REACH Regulation you should revise the PBT assessment when results of the tests detailed above are available.

5. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

In accordance with Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to IX to the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.
"Bioaccumulation in aquatic species, preferably fish" is a standard information requirement as laid down in Annex IX, Section 9.3.2.of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt the information requirement of Annex IX, Section 9.3.2.of the REACH Regulation and provided the following justification for the adaptation:

> *"The registration substance is a multi-constituent and due to the strongly basic nitrogen atoms present in the different constituents (pKa_1 12.7-14.7 and pKa_2 10.1-13.8, see IUCLID Chapter 4.21) a cationic surfactant. Due to the estimated pKa it is obvious that in the environmental pH range of 4 to 9 the constituents are mono- or di-protonated. The property estimation program US EPA KOWWIN Version 1.68 allows to calculate the Log Kow for the different mono- or di-protonated constituents. The estimated Log Kow values are in the range of -7.5 and 2.8. For the highest Log Kow of 2.8 the US EPA BCFBAF model Version 3.01 calculates a BCF of 31 L/kg wwt (Regression model) and 38 L/kg wwt (Arnot-Gobas model) which means a low potential for bioaccumulation. For (cationic) surfactants classical measurements like shake-flask (OECD 107), HPLC (OECD 117) or Slow stirring (OECD 123) are not suitable as the result depends form the measurement conditions. Instead the Log Kow may be estimated from the solubility in 1-Octanol and the CMC (Critical micelle concentration). The registration substance is miscible in 1-Octanol in every proportion but this may not reflect the true solubility of the single constituents as the solubility of the mixture is influenced by the various constituents (co-solvency). The Log Kow calculated from the 1-Octanol solubility and the CMC of the registration substance is 3.6 at 20 degree Celsius (see IUCLID Chapter 4.7). This is higher than the highest Log Kow calculated for the different protonated constituents of the registration substance. It is below the 'B' criteria of log Kow >4.5 for the PBT / vPvB Assessment. Based on the Log Kow of 3.6 the Exposure modelling program EUSES calculates a BCF fish of 229 L/kg wwt which is below the 'B' criteria of >2000 for the PBT /vPvB Assessment.*

CONCLUSION: Based on the measured as well as the estimated Log Kow given above, the registration substance is not bioaccumulative. It is important to note that cationic surfactants strongly sorb to negatively charged surfaces like clays and glass but also to biota (e.g. fish mucous). These properties make a BCF fish study for the registration substance according OECD 305 infeasible".

ECHA notes that the justification for your adaptation is threefold:

a) you claim that based on the log Kow value, estimated or measured, the substance has a low potential for bioaccumulation;
b) you claim that QSAR models, either the US EPA BCFBAF or EUSES, predicts BCF values that are below the 'B' criterion for the PBT/vPvB assessment;
c) you claim that an experimental study according to OECD test guideline 305 is not feasible.

a) The bioaccumulation is not correlated to log Kow for surfactant

Column 2 of Section 9.3.2. of Annex IX of the REACH Regulation specifies that a bioaccumulation study need not be conducted if "*the substance has low potential for bioaccumulation (for instance a log Kow ≤ 3) and/or a low potential to cross biological membrane*" or if "*direct and indirect exposure of the aquatic compartment is unlikely*".

The registered substance is a cationic surfactant. By design, cationic surfactants contain two distinct moieties, a hydrophilic (cationic) headgroup and a hydrophobic tail. Consequently, they tend to adsorb at the interfaces of the aqueous and lipid phases. For this reason, it is difficult to obtain a reliable log Kow value for such substances. ECHA's Guidance on Information Requirements and Chemical Safety Assessment, chapter R7a (version 6.0, July 2017), proposes as an alternative to compare measured solubilities in octanol and water, using the critical micelle concentration in water (CMC) as a solubility limit in water, or to use predictions from validated QSARs. However log Kow may as such not be suitable for the determination of the bioaccumulation potential of surfactants (ECETOC, 2014)[4]. The bioaccumulation of surfactants in fish actually shows no correlation with log Kow. On one hand, many linear alkyl chain surfactants are readily biotransformed in fish, so that the actual bioaccumulation may be lower than predicted from log Kow. On the other hand, surfactants may adsorb to food and can contribute to an increased intake via the diet, independently of the log Kow of the substance (Treu et al. 2015)[5]. Cationic surfactants will in particular tend to bind to negatively charged sites like fish mucous. Equilibrium and depuration are expected to be retarded for such substances. Therefore, ECHA considers that log Kow is not a suitable parameter to assess the bioaccumulation potential of the substance and threshold values based on log Kow, e.g. those defined for the 'B' and 'vB' criteria, should be regarded as not applicable to surface-active substances.

ECHA further notes that the substance is used as disinfectant with wide-dispersive uses and expected to be releases to water. Exposure to the aquatic compartment is therefore likely.

ECHA therefore considers that the specific rules for adaption of column 2 of Annex IX, Section 9.3.2. of the REACH Regulation are not met.

[4] ECETOC, 2014. Information to be considered in a weight-of-evidence-based PBT/vPvB assessment of chemicals (Annex XIII of REACH) Special Report No. 18. Eureopean Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC).
[5] G. Treu, W. Drost, U. Jöhncke, C. Rauert and C. Schlechtriem, 2015. The Dessau workshop on bioaccumulation: state of the art, challenges and regulatory implications. Environmental Sciences Europe. 27:34

b) Qualitative or Quantitative Structure-Activity Relationship ((Q)SAR) (Annex XI, Section 1.3.)

Article 13(1) of the REACH Regulation provides that information on intrinsic properties of substances may be generated by means other than tests, "*provided that the conditions set out in Annex XI are met*". This annex proposes some general rules for adapting the standard information requirements set out in Annexes VII to X of the REACH Regulation.

In particular, Annex XI, Section 1.3. of the REACH Regulation introduces the concept of Qualitative or Quantitative Structure-Activity Relationship ((Q)SAR) as another possible general rule for adapting the standard information requirements set out in Annexes VII to X of the REACH Regulation. Annex XI, Section 1.3. of the REACH Regulation specifies that (Q)SAR results may be used instead of testing if the following conditions are met:

- "*results are derived from a (Q)SAR model whose scientific validity has been established,*
- *the substance falls within the applicability domain of the (Q)SAR model,*
- *results are adequate for the purpose of classification and labelling and/or risk assessment, and,*
- *adequate and reliable documentation of the applied method is provided*".

In your justification, you make reference to BCF values calculated with different pieces of software: US EPA BCFBAF and EUSES. However both programs estimate the BCF of the substance using a log Kow value. As explained in section 5(a) above, log Kow is considered to be not suitable for the prediction of the bioaccumulation of surface-active substances. For example, in EUSES, in the absence of experimental data for bioaccumulation, it is recommended for surface-active substances to use a worst-case approach (P. van Beelen, 2000)[6]. The Arnot-Gobas model[7], which is part of the US EPA BCFBAF program, further includes the estimation of a biotransformation rate in fish but still heavily relies on log Kow to predict BCF. For this reason, this model should not be used for surface-active substances[8].

Therefore ECHA considers that the scientific validity and the applicability of the bioaccumulation models included in US EPA BCFBAF or in EUSES have not been established for surface-active substances.

Based on the explanation above ECHA considers that the general rules for adaptation of Annex XI, Section 1.3. are not met.

c) Technical feasibility of the bioaccumulation study (Annex XI, Section 2.)

Annex XI, Section 2. of the REACH Regulation provides some provisions for substances for which testing is technically not possible because of the properties of the substance.

In your justification, you finally claim that "*cationic surfactants strongly sorb to negatively charged surfaces like clays and glass but also to biota (e.g. fish mucous)*" and that "*these*

[6] P. van Beelen, 2000. The risk evaluation of difficult substances in USES 2.0 and EUSES. A decision tree for data gap filling of Kow, Koc and BCF. RIVM report 679102050
[7] J. A. Arnot and F. A. P. C. Gobas, 2003. A Generic QSAR for Assessing the Bioaccumulation Potential of Organic Chemicals in Aquatic Food Webs. QSAR Comb. Sci. 22
[8] The authors of this model themselves recommend that it should be applied with great care to ionisable or surface-active substances (Arnot and Gobas, 2003)

properties make a BCF fish study for the registration substance according OECD 305 infeasible".

The latest version of the OECD 305 test guideline proposes two routes of exposure, either an aqueous exposure (part-I of the test guideline) or a dietary exposure (part III of the test guideline). For surface active substances, the OECD 305 test guideline indicates that "*it should be considered whether the aqueous bioconcentration test is feasible, given the substance properties, otherwise the dietary study is probably more appropriate. Surfactants are surface acting agents, which lower the interfacial tension between two liquids. Their amphiphilic nature (i.e. they contain both a hydrophilic and a hydrophobic part) causes them to accumulate at interfaces such as the water-air interface, the water-food interface, and glass walls, which hampers the determination of their aqueous concentration*". Cationic surfactants will in particular tend to bind to negatively charged sites like indeed clays, glass and biota (i.e. not only the test fish but also food items). ECHA notes that laboratory glassware can be treated to avoid excessive adsorption, e.g. by soaking it with aqueous solutions of the surfactant overnight, then rinsing successively with different solvents, or by using special glassware (Schmitt, 2001)[9]. However, as the registered substance is expected to adsorb also onto food, intake via the diet needs to be considered. Therefore ECHA considers that part III of OECD test guideline 305 (the 'Dietary Exposure Bioaccumulation Fish Test') is not only feasible but also relevant for assessing the bioaccumulation potential of the registered substance.

Therefore, ECHA considers that a bioaccumulation study is technically feasible and that the general rules for adaptation of Annex XI, Section 2. are not met.

d) Outcome

As explained above, you have sought to adapt the information requirement of Annex IX, Section 9.3.2.of the REACH Regulation for "Bioaccumulation in aquatic species". ECHA considers that your adaptations neither meet the specific rules for adaptation of column 2 of Annex IX, Section 9.3.2. of the REACH Regulation, nor the general rules for adaptation of Annex XI of the REACH Regulation. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7c* (version 3.0, June 2017) bioaccumulation in fish: aqueous and dietary exposure (test method OECD TG 305) is the preferred test to cover the standard information requirement of Annex IX, Section 9.3.2.

As explained above, the registered substance is a surfactant and ECHA acknowledges that it may be difficult to follow aqueous concentrations. Besides, as the substance is expected to adsorb strongly onto food, the intake via the diet needs to be considered. Therefore ECHA considers that a dietary exposure bioaccumulation fish test (part III of the test guideline) is more suitable than an aqueous exposure test.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Bioaccumulation in fish: dietary exposure bioaccumulation fish test (test method: OECD TG 305-III)

[9] T.M. Schmitt, 2001. Analysis of Surfactants, Second Edition. CRC Press.

Notes for your consideration

Before conducting the above test you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment*, Chapter R.11.4. and Figure R.11-4 on the PBT assessment (version 3.0, June 2017) for further information on the integrated testing strategy for the bioaccumulation assessment of the registered substance. You should revise the PBT assessment when information on bioaccumulation is available.

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 1 March 2017.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA did not receive any comments by the end of the commenting period.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

ECHA received proposal(s) for amendment and modified the draft decision.

ECHA invited you to comment on the proposed amendment(s).

ECHA referred the draft decision to the Member State Committee.

You did not provide any comments on the proposed amendment(s).

The Member State Committee reached a unanimous agreement on the draft decision in its MSC-57 written procedure and ECHA took the decision according to Article 51(6) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks on the present registration at a later stage.

2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

3. In relation to the information required by the present decision, the sample of the substance used for the new tests must be suitable for use by all the joint registrants. Hence, the sample should have a composition that is suitable to fulfil the information requirement for the range of substance compositions manufactured or imported by the joint registrants.

   It is the responsibility of all joint registrants who manufacture or import the same substance to agree on the appropriate composition of the test material and to document the necessary information on their substance composition. In addition, it is important to ensure that the particular sample of the substance tested in the new tests is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured or imported by each registrant.

   If the registration of the substance by any registrant covers different grades, the sample used for the new tests must be suitable to assess these grades. Finally there must be adequate information on substance identity for the sample tested and the grades registered to enable the relevance of the tests to be assessed.