EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004198-69-03/F Helsinki, 18 August 2014

DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006

For Naphtha (petroleum), full-range alkylate, CAS No 64741-64-6 (EC No 265-066-7), registration number: [redacted]

Addressee: [redacted]

The European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 51 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

I. Procedure

Pursuant to Article 41(1) of the REACH Regulation ECHA has performed a compliance check of the registration for Naphtha (petroleum), full-range alkylate, CAS No 64741-64-6 (EC No 265-066-7), submitted by [redacted] (Registrant). The scope of this compliance check is limited to the standard information requirements of Annex I, Section 3.3.1. of the REACH Regulation, specifically to predicted no effect concentrations (PNECs) freshwater and marine water. ECHA stresses that it has not checked the information provided by the Registrant and other joint registrants for compliance with requirements regarding the identification of the substance (Section 2 of Annex VI).

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band of 1000 tonnes or more per year. The registration was made by the Registrant for on-site isolated intermediate uses under strictly controlled conditions while he submitted the registration dossier as lead registrant on behalf of all member registrants covering as well non-intermediate uses that are subject to compliance checks.This decision does not take into account any updates submitted after 8 May 2014, the date upon which ECHA notified its draft decision to the Competent Authorities of the Member States pursuant to Article 51(1) of the REACH Regulation.

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

The compliance check was initiated on 3 September 2013.

On 18 October 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision.

On 14 November 2013 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments. On basis of this information, only the deadline in Section II was amended. Comment on classification and labelling provided by the Registrant is addressed in the Statement of Reasons (Section III).

On 08 May 2014 ECHA notified the Competent Authorities of the Member States of its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals for amendment of the draft decision within 30 days of the receipt of the notification.

As no proposal for amendment was submitted, ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

II. Information required

Pursuant to Articles 41(1)(c), 41(3), 10(b), 14 and Annex I of the REACH Regulation the Registrant shall submit in the chemical safety report (CSR) and in section 6 of the technical registration dossier (IUCLID):

> Revised predicted no effect concentrations (PNECs) for freshwater and marine water as specified in the Statement of reasons (section III) (Annex I, 3.3.1. of the REACH Regulation).

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by **25 February 2016**.

III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein, submitted by the Registrant for registration of the above mentioned substance for the purpose of registration within the applicable tonnage band of 1000 tonnes or more per year in accordance with Articles 6 and 11(1) of the REACH Regulation, does not comply with the requirements of Articles 10(b), 13 and 14 or with Annexes I and XI thereof. Consequently, the Registrant is requested to submit the information mentioned above that is needed to bring the registration into compliance with the relevant information requirements.

Non-compliance of PNECs freshwater and marine water

In accordance with Annex I, 3.3.1. of the REACH Regulation, a PNEC for each environmental sphere shall be established based on the available information and shall be reported in the CSR. While the Registrant has reported experimental key studies in the IUCLID file in section 6, the results of these key studies are not used for deriving PNEC values. Therefore, ECHA considers the experimental studies reported in IUCLID as supporting studies. ECHA notes that the PNEC may be calculated by the Registrant by different means as long as the available data is taken fully into consideration.

The PNEC values used in the risk assessment in the registration dossier are derived from environmental risk assessment IT tools, namely the PETROTOX/PETRORISK IT tools, with an applied assessment factor of 1. PETROTOX is a quantitative structure-activity relationship ((Q)SAR) tool based on the target lipid model (TLM) which predicts the toxicity of petroleum products to aquatic organisms. PETRORISK is a tool that performs environmental risk assessment incorporating the effect values predicted by PETROTOX via the TLM.

As the effect values used in PNEC derivation are derived using the above mentioned (Q)SAR models, and not on the basis of the experimental key studies available to the Registrant for the registered substance subject to the present decision, ECHA considers that the Registrant has chosen to adapt the relevant standard information requirements which are necessary for environmental hazard assessment. The environmental hazard assessment has to be carried out in accordance with Annex I, section 3. of the REACH Regulation.

By employing (Q)SARs the Registrant has to meet the respective requirements in order to replace the available test data.

Annex XI, section 1.3. sets out the conditions which must be fulfilled in order for the results of (Q)SARs to be acceptable as a replacement for experimental studies:

- 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.

ECHA considers that the results from the application of the PETRORISK/PETROTOX tools fail to meet the first condition above as the scientific validity of these tools, and in particular the target lipid model upon which the tools are based, has not been sufficiently established. Consequently, the PETRORISK/PETROTOX tools are not suitable for classification and labelling and/or risk assessment.

The Registrant commented the draft decision stating that the PETROTOX tool would never be used for the purpose of classification and labelling that would always be based on experimental data using a worst case approach. ECHA acknowledges this clarification and notes that adequacy for the purpose of classification and labelling and/or risk assessment is a standard condition for the use of (Q)SAR data in place of testing in accordance with Annex XI, section 1.3. as outlined above.

PETRORISK and PETROTOX in their current form are considered as not scientifically valid for the following reasons[1]:

1. the insufficient number of taxonomic groups used in the acute and chronic Species sensitivity distributions (SSDs),
2. shortcomings in the acute-to-chronic ratio (ACR) derivation,
3. shortcomings in the HC5 derivation: the assumption of a normal distribution, which is not met for log CTLBB (critical target lipid body burden) and log ACR (acute to chronic ratio) and the assumption of independent parameters, which is not met for the combination of CTLBB and the universal slope for narcosis,
4. omission of phototoxicity effects of PAHs,
5. underestimation of chronic toxicity when compared with data from experimental studies.

Consequently ECHA considers that there is an inconsistency between the available experimental data not used in the PNEC derivation and the reported PNECs derived from the PETRORISK/PETROTOX tools and that the PNECs in the registration dossier for freshwater and marine water are not valid. Hence, new PNECs shall be derived taking into account the discrepancies outlined above and specified further as follows:

[1] Emiel Rorije, Eric M.J. Verbruggen & Joop A. de Knecht. Service Request on a critical review of the environmental and physicochemical methodologies commonly employed in the environmental risk assessment of petroleum substances in the context of REACH registrations (05 August 2012, Version 4).

1. Species sensitivity distribution on acute data

It should be noted that although the SSD contains 47 species, there is no higher aquatic plant (macrophyte) or blue-green algae (cyanophyte) included. Both are important organism goups. According to the REACH guidance[2] the minimum species requirements when using the SSD method are fish, a second family in the phylum *Chordata*, a crustacean, an insect, a family in a phylum other that *Arthropoda* or *Chordata*, a family in any order of insect or any phylum not already represented, algae and higher plants. Because higher plants belong to the eight taxonomic groups defined as minimum requirement to perform a SSD this minimum number of taxonomic groups is thus not met. Therefore, although CTLBBs are present for 47 species, the Registrant did not justify why the SSD approach with less than required taxonomic groups would still be acceptable.

2. Acute to chronic ratio (ACR)

A number of aspects lead to an underestimation of the ACR in PETRORISK/PETROTOX:

- It is noted that in case real acute effects were not observed in the studies, behavioural effects were used instead in deriving the ACR used in the IT tools. Behavioural effects occur at lower concentrations than the standard acute endpoints such as mortality, immobility or population growth and consequently will lead to an underestimation of the ACRs. Importantly, because these behavioural effects are not considered in the construction of the target lipid model, it is also not appropriate to use ACRs which are derived based on these effects.
- Overall, the distribution of ACR values used for petroleum substances in the target lipid model does not cover the full range of available ACR values (e.g. the high ACRs for some crustaceans are not taken into account). Therefore, the ACR taking into account all available information[3,4] (including the high ACRs) will lead to a higher ACR than the one used in the IT tools as presented by the Registrant. Consequently the chronic toxicity may be underestimated.
- According to the REACH guidance[5] the minimum species requirements when using the SSD method are fish, a second family in the phylum *Chordata*, a crustacean, an insect, a family in a phylum other that *Arthropoda* or *Chordata*, a family in any order of insect or any phylum not already represented, algae and higher plants. The ACRs available in the IT tools cover eleven species (two algal, three crustacean, four fish, one insect, and one rotifer species). Therefore, the number of species (marginally) meets the REACH guidance requirements for using a chronic SSD: "*...at least 10 NOECs (preferably more than 15)...* " However, the conditions for using a chronic SSD regarding the number and type of taxonomic groups are not met as this set is lacking 2 of the 8 required taxonomic groups "*a family in any order of insect or any phylum not already represented*" and "*higher plants*".
- A comparison of the mean (3.83) and 95th percentile (13) ACRs derived in the TLM with the ACRs derived from experimental data on polycyclic aromatic hydrocarbons (PAH) showed that a substantial number of these PAH ACRs are above the TLM's 95th percentile ACR (i.e. >13) [5]. Therefore, the mean and 95th percentile ACR used in the TLM is not protective for at least these PAHs.

[2] ECHA guidance on information requirements and chemical safety assessment, chapter R.10.3.1.3. (May 2008).
[3] Emiel Rorije, Eric M.J. Verbruggen & Joop A. de Knecht. Service Request on a critical review of the environmental and physicochemical methodologies commonly employed in the environmental risk assessment of petroleum substances in the context of REACH registrations (05 August 2012, Version 4).
[4] Verbruggen *et al.*, 2008; Ahlers *et al.*, 2006; Raimondo *et al.*, 2007.
[5] ECHA guidance on information requirements and chemical safety assessment, R.10.3.1.3. (May 2008).

3. Equation used to arrive at a HC5 (hazardous concentration for 5% of species)

For the equation to calculate HC5 to be correct the individual parameters for which the uncertainty is accounted for should be independent of each other and should be log normally distributed. However, the assumption of independence of parameters is not met for the combination of CTLBB and the universal slope for narcosis[3]. For the intercept, the variance is only based on the variance in estimated CTLBBs. However, the variance in the intercept is correlated to the variance of the slope as well (i.e. the higher the slope, the lower the intercept). On top of that, the general intercept of the relationship between the logarithms of K_{mw} and K_{ow} is now assumed to be zero but should be added to these CTLBBs. This intercept has its own variance and is also not independent of the universal slope. Furthermore, two of the three parameters used in the equation (slope, CTLBB, and ACR) do not follow a log normal distribution. The SSD on the CTLBB does not follow a normal distribution as expected, and the ACR should not be normally distributed based on theoretical considerations, although the choice of data for this parameter is probably more influential on the final result. Therefore, the requirement that the parameters are normally distributed is not met. Essentially, the equation which is used to derive the HC5 which is subsequently used to derive the PNECs is not scientifically valid as the fundamental assumptions made in its derivation have been shown to be incorrect.

4. Phototoxicity of PAHs (polycyclic aromatic hydrocarbons)

The assumed mode of toxic action of petroleum substances is narcosis. Although the mechanism of chronic toxicity could be different, the general assumption in the PETRORISK/PETROTOX IT tools is to base the toxicity on internal target lipid concentrations. However, it appears that phototoxicity of PAHs is a toxic acute effect, with effect concentrations (EC50s) at similar levels as the lowest chronic no-observed effect concentrations (NOECs). Although phototoxicity in petroleum products as a whole will not be as extreme as for some of the individual PAHs, the occurrence of phototoxicity for petroleum products has been demonstrated[3]. In the target lipid model phototoxic effects were not considered at all. However, this specific mode of action should have been separated from the general assumption of narcosis and should have been covered in the model.

5. Comparison of the HC5 with experimental chronic data

The target lipid model has been compared with a limited number of chronic toxicity studies on petroleum compounds[6]. The chronic HC5 levels are higher than HC5 values derived directly from experimental data for individual substances and HC5 values derived in a comparable way from chronic toxicity data for PAHs and petroleum products. Some reasons for this discrepancy are the selection of ACRs and the dependency of the parameters CTLBB and universal slope for narcosis as explained above. Also a comparison between the chronic values derived with the TLM used in the PETROTOX/PETRORISK IT tools and chronic toxicity data from experimental studies showed some differences. In general, acute toxicity of monoaromatics, polycyclic aromatic hydrocarbons, and oil and PAH mixtures were fairly well predicted, with the accuracy within a factor 3 to 5. For chronic toxicity, however, the results were more variable and the toxicity has been shown to be underestimated by up to a factor

[6] Emiel Rorije, Eric M.J. Verbruggen & Joop A. de Knecht. A critical review of the environmental and physicochemical methodologies commonly employed in the environmental risk assessment of petroleum substances in the context of REACH registrations. 05 August 2012, Version 4.

of 44. This indicates that the TLM used in the PETROTOX and PETRORISK IT tools in their present form, with the errors outlined above is not a conservative or protective approach for all relevant substances. Importantly, the Registrant did not provide a thorough validation of the PETROTOX/PETRORISK IT tools with high quality experimental acute and chronic data.

ECHA notes that the justification for applying an assessment factor of 1 to the chronic HC5 when deriving the PNEC is not sufficient and does not address all of the uncertainties linked with the PNEC value. In accordance with Annex I, 3.3.1. of the REACH Regulation a PNEC may be calculated by applying an appropriate assessment factor to the effect values. Given the variable composition of many petroleum substances and the uncertainty associated with mass distribution over hydrocarbon blocks and considering also the uncertainty attached to the number and the physico-chemical properties of individual constituents of the library included in the PETROTOX/PETRORISK IT tools to represent petroleum substances this assessment factor is not substantiated. Furthermore, Oxygen and Nitrogen containing petroleum substances are absent from the library of structures in the PETROTOX/PETRORISK IT tool and the uncertainty linked to this omission has not been addressed by the Registrant in the registration dossier in the context of assessment factor selection.

On the basis of the above considerations, the Registrant is requested to submit the required information as set out in section II in an updated registration dossier.

IV. Deadline for submitting the required information

In the draft decision communicated to the Registrant the time indicated to provide the requested information was 6 months from the date of adoption of the decision. ECHA has taken note of the significant investigations proposed in the action plan to address the draft decision issues and considers that 18 months from the date of adoption of the decision is a reasonable time period for providing the required information in the form of an updated dossier. The decision was therefore modified accordingly.

V. Information on right to appeal

An appeal may be brought against this decision to the Board of Appeal of ECHA under Article 51(8) of the REACH Regulation. Such an appeal shall be lodged within three months of receiving notification of this decision. Further information on the appeal procedure can be found on ECHA's internet page at http://echa.europa.eu/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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