

CEFIC Long-Range Research Initiative Request for Proposals (RfP)

Title and Code Number:

Applying and verifying PBT/POP models through comprehensive screening of chemicals – ECO13

Background

PBT/POPs are a specific group of chemicals with a combination of properties that give rise to additional concern and to increased uncertainty in assessing their risks. During the last decade a number of PBT/POP models have come to the stage where they can be applied in practice with sufficient reliability for certain substances and purposes. These models are now starting to be used in regulatory contexts.

Appropriate scientific screening, identification and assessment to distinguish PBT/POPs from 'other' chemicals require a number of steps applying a range of methodologies and verification through monitoring. If a large group of chemicals is analysed to identify PBT/POPs by applying inadequate screening methods or an insufficient number of screening or assessment steps, there is a high risk of erroneous conclusions and unfounded concern about the number of potentially hazardous substances. Applying and verifying PBT/POP models for adequate and extensive screening of a comprehensive list of substances relevant for the EU market for high potential impact and subsequent verification of the findings through monitoring can be of great value.

Finally a more in-depth further assessment of potential impact and actual risks, including production volumes, emissions, detailed exposure, critical effect levels, etc. will be needed, but this is outside the scope of the present project.

References

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F Wania, The global distribution model. A non-steady state multi-compartmental mass balance model of the fate of persistent organic pollutants in the global environment. Technical report and computer programme, **2000**, 21 pp., (www.uts.utoronto.ca/~wania).

F Wania, Assessing the potential of persistent organic pollutants for long-range transport and accumulation in polar regions, *Environ. Sci. Technol.* **2003**, *37*, 1344-1351.

F Wania, Potential of degradable organic chemicals for absolute and relative enrichment in the Arctic, *Environ. Sci. Technol.* **2006**, *40*, 569-577.

MS McLachlan, K Breivik, T Brown, G Czub, F Wania, Screening for potential contaminants in Arctic food chains. Application of a linked non-steady-state chemical fate and bioaccumulation model, Poster LRI Workshop November 2007.

F Wania, NJ Persson, MS McLachlan, CoZMo-POP 2 – A fugacity-based dynamic multi-compartmental mass balance model of the fate of persistent organic pollutants, *Environ. Model. Software* **2006**, *21*, 868-884.

Objectives

1. To apply a combination of relevant 'screening filters' and advanced quantitative PBT/POP models including food-chain accumulation, to a broad list of chemicals relevant for Europe to demonstrate a science-based approach for identifying

- substances with a high potential to accumulate in local and/or remote environmental compartments and biota.
2. To verify the outcome of objective #1 by analysing existing measured data and carrying out additional measurements in appropriate compartments. Additional measurements should preferably be done within the context of existing and reliable monitoring networks to benefit from transport, sampling and quality assurance infrastructure.
 3. The deliverables would be a detailed verification of models as a result of the combined objectives #1 and #2 with recommendations for their use. An additional deliverable may be recommendations for further evaluation of the potential impact of identified substances with a potential high concern.

Scope

The screening should start from a list as broad as possible, but manageable. Preferably the full EU list of HPVs (High Production Volume chemicals, i. e. >1000 t/y) and LPVs (Low Production Volume) should be used as a starting point. Then modelling and screening (filter) steps should be carried out, preferably applying publicly available models, for example those which have been (co-)developed within the LRI Programme, i.e. CoZMo-POP, ACC-HUMAN, or IMPS. The screening steps could involve several physico-chemical properties, characteristics like long-range transport potential, degradation rates, etc. The screening, filtering and advanced modelling process should apply as many relevant tools as possible to reach a limited and realistic final priority set of substances for further in-depth investigation. Subsequently, these priority substances should be evaluated in more detail to identify relevant and non-relevant substances for further verification/validation. Verification and validation through monitoring should select appropriate geography, appropriate environmental compartments (including biota) and preferably work in close cooperation with well-known existing monitoring networks to benefit from existing and well performing logistics, such as access to sites, sampling and quality compliance procedures. Finally, further evaluation steps could be recommended.

Short interim reports on progress are required at 6-monthly intervals. It is expected that the findings will be developed into a peer reviewed publication, following presentation at a suitable scientific conference.

Cost and Timing

Budget in the order of €400,000

Start in 2008, duration up to 36 months