ACCOUNTING FOR PHOTO DEGRADATION IN THE PBT ASSESSMENT OF CHEMICALS

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INTRODUCTION and OBJECTIVES

Photo degradation (PhoDeg) in water may be an important removal mechanism of chemical substances from the environment, in particular for chemicals that resist biodegradation. Two main mechanisms of photolysis have been described in the aquatic environment: (1) Direct photolysis, occurring when a given chemical absorbs light and as a consequence of that absorption undergoes transformation. (2) Indirect photolysis, occurring either when another excited species transfer their energy to the chemical (sensitized photolysis) or when reactive (non-excited) compound present in the media (e.g. hydroxyl radicals) react with the chemical. Photo reactivity of chemicals cannot be estimated from chemical structure by means of QSARs. PhoDeg rates in water are obtained from laboratory measurements. Information on PhoDeg in water is often neglected in P- assessment of chemicals, due to lack of systematic procedures to translate such information into "half-lives in water". However, REACH regulation requires that chemical substances be assessed with respect to persistence, bioaccumulation and toxicity (PBT). The REACH Guidance specifies an Integrated Testing Strategy for carrying out persistence assessments indicating that Information on PhoDeg may be used in the assessment of (non) persistence. Although the spirit of the regulation is clear, still unclear how to deal with some specific issues: (1) Extrapolation of measured PhoDeg rates in water under laboratory conditions to half-lives in natural water. (2) Definition of relevant environmental characteristics for evaluating "half-lives in water". (3) Identification of environmental compartments which need to be considered "relevant". The OBJECTIVES of the present work are to evaluate and apply the current knowledge on quantitative description/prediction of PhoDeg rates in water and to propose a modeling procedure to account for photo degradation in P assessment of chemicals.

APPRAOCH

A: Peer-reviewed scientific literature screening
- SCOPUS keyword search (1990-2009), 120 publication selected and 80 examined in detail (critical review)
- PhoDeg rates dependence on environmental variables (e.g. water pH or DOM)
- Type of information on PhoDeg that may be used in P assessment.

B: Revision of main official methods dealing with direct photo-transformation of chemicals in water
- OECD/DG(9721 and OECD 315)
- US EPA OPPTS 830.210

C: Revision of main algorithms used to account for PhoDeg in environmental fate models
- Exposure Analysis Modeling System (EXAMS)
- Marine Antifoulant Model to Predict Environmental Concentrations (MAMPEC)

CONCLUSIONS AND RECOMMENDATIONS

Quantitative knowledge of the rate of photo degradation in water can be applied for the purpose of P-assessment under REACH as follows:

- Rates of direct photolysis in clear water can be obtained by standard procedures and should be made available from registration dossiers.
- The influence of DOM on direct photolysis can be accounted for
- The influence of DOM on indirect PhoDeg and the influence of pH can be accounted for only if experimental knowledge is available.
- PhoDeg in natural waters is much slower than in clear (laboratory) water: ~15-~/400 and ~50-300μm in typical fresh, coastal sea and ocean water, respectively.
- For the purpose of P-assessment, "half-life in water" can be derived as the weighted average of half-lives in the various water types typically modeled in environmental risk assessment of chemicals, using modeled steady-state mass fractions in the various waters as weighting factors.