

Linking algal growth inhibition to chemical activity - DTU Orbit (08/11/2017)

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Unitless chemical activity, expressing the energetic level of a compound relative to its energetic level in pure liquid [0-1], has proven useful to quantify the effective exposure to hydrophobic organic compounds through both aerial and aqueous media. Several studies have linked toxicity to chemical activity, as opposed to e.g. the total concentration. Baseline toxicity (narcosis) for neutral hydrophobic organic compounds has been shown to initiate in the narrow chemical activity range of 0.01 to 0.1. This presentation focuses on linking algal growth inhibition to chemical activity with the aims to (1) further challenge the current chemical activity range for baseline toxicity, and (2) extend the utilisation of the chemical activity concept across compounds and species. The first part of the presentation focuses on results from a recently published study, in which toxicity data for 39 non-polar liquids were applied to challenge the chemical activity range for baseline toxicity. For each compound, the effective activity (Ea_{50}) was estimated as the ratio of the effective concentration (EC_{50}) and water solubility. Of these ratios, 90% were within the expected chemical activity range of 0.01 to 0.1 for baseline toxicity, and none of the ratios were significantly below 0.01. On a practical level, these findings suggest EC_{50} values for baseline toxicity to be at or above 1% of water solubility. On an environmental risk assessment level, predicted no-effect concentrations (PNECs) for baseline toxicity could even be set as a percentage of saturation, and this approach can easily be extended to baseline toxicity of mixtures. However, EC_{50} values well below 1% of saturation can still occur and indicate the potential for excess toxicity through a specific or reactive mode of action. The second part of the presentation focuses on extending the utilisation of the chemical activity concept. More specifically, the chemical activity concept is applied to a much larger range of algal toxicity data, including a wide range of solids and liquids, covering several expected modes of action and also several algal species. High-quality toxicity data are carefully selected from peer-reviewed scientific literature and QSAR databases. This presentation shows how the chemical activity concept can be used to compare and combine toxicity data across compounds and species in order to characterize toxicity – and further how the concept can be used in environmental risk assessment.

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Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University

Authors: Schmidt, S. N. (Ekstern), Mayer, P. (Intern)

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