

Predictions of the Aquatic Toxicity of High-Production-Volume-Chemicals

Part A: Introduction and Methodology



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11 Summary In this report, QSAR estimates are presented for the aquatic toxicity of High Production Volume Chemical (HPVCs) from the European Inventory (EINECS). Around 48% (977 chemicals) of the HPVCs could be classified. It appears that a little over 1000 HPVCs fall into non-classifiable categories as inorganics? polymers and ill-defined mixtures (e.g. petroleum products). For 230 HPV chemicals reliable estimates could be made for acute and chronic toxicity to fish and Daphnia, toxicity to algae and no-effect levels at the ecosystem level for surface water and sediments. For other classes of HPV chemicals, only worst case estimates for acute toxicity to fish are presented. The predictions are based on the current status of predictive models, which were discussed in the OECD Hazard Assessment Advisory Body. The report consists out of two parts. Part 1 gives an outline of the predictive methodologies and in part 2 the predictions of aquatic effects for the HPVCs are listed.		
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Summary

In this report, QSAR estimates are presented for the aquatic toxicity of a sub-set of the High-Production-Volume Chemicals (HPVCs) from the **European** Inventory of New **and** Existing Chemicals (EINECS). The predictions are **based** on:

- A scheme to **classify** chemicals into four different classes based on their chemical structure
- A set of QSAR equations for different endpoints of ecotoxicity
- Extrapolation methods for calculation of **safe** levels at the ecosystem level (**HC₅ values**)
- An equilibrium partitioning model for calculating **HC₅** values for sediment

Around 48% (**977** chemicals) of the HPVCs **could** be classified according to this scheme. It appears that a little **over 1000** HPVCs fall into non-classifiable **categories** as inorganics, polymers and ill-defined mixtures (e.g. petroleum **products**).

The subset of **class 1** chemicals, which **consists** of **230** HPV chemicals, represent those chemicals that **can** be classified as '**inert** chemicals'. The estimated parameters for these **narcotic** chemicals **include: acute** and chronic toxicity to fish and daphnids, toxicity to algae, and no-effect levels at the ecosystem level for surface water and sediments. For other classes of HPV chemicals, only worst case estimates for **acute** toxicity to fish are presented.

The predictions are based on the **current** status of predictive models. Future studies are planned to improve the models for ecotoxicity and fate processes. These improved models **will** also be applied to the HPVCs. This **activity will be carried out** within the **framework** of an international project **funded** by the **European** Communities (DG-XII). The report **consists** of two parts:

Part A gives an outline of the predictive methodologies and also **contains** the necessary background information in the form of original publications of a number of **referenced** papers.

Part B includes tables with the **actual** predictions of aquatic **effects** for the HPVCs.

Introduction

The EC Council Regulation on the evaluation and control of the **environmental** risks of existing substances [1] **has** recently been adopted and applies to the collection, distribution and **accessibility** of information on existing substances. It **includes** the evaluation of the risks of existing substances to man, including workers and **consumers**, and to the environment, in order to **ensure** better management of those risks within the framework of Community provisions.

One article (Article 3) is **devoted** to so-called High Production Volume Chemicals (HPVCs). Any manufacturer who **has** produced or any importer who **has** imported an existing substance, as **such** or in a **preparation**, in quantities exceeding **1000** tons per year, must submit information to the Commission at **least** once every three **years**. This information is listed in Table 1. Similar **activities** are **taking** place in a number of other OECD member countries.

Table 1. Required information for HPVCs

the name of the substance
the quantity of the substance produced or imported
the classification of the substance according to Directive 67/548/EEC
information on the reasonable foreseeable uses of the substance
data on the physicochemical properties of the substance
data on pathways and environmental fate
data on the ecotoxicity of the substance
data on the acute and subacute toxicity of the substance
data on carcinogenicity, mutagenicity and/or toxicity to reproduction
other indications relevant to the risk evaluation of the substance

Attention **will** be focused on the approximately **2000** HPVCs which are listed in Annex 1 of the Council Regulation. In Annex II of the Council Regulation a set of data is described that is considered to be **sufficient** for priority setting and initial **hazard** assessment of chemicals. This data set **will** have to be **filled** with available information by **manufacturers**.

It is expected that for the **2000** HPVCs, **many** data gaps **will** be found. **Predictions** of the data availability **by European** experts, including representatives from the industry, are given in Table 2[2]. From this table it **can** be concluded that **fully** completed **HEDSETs** with **Annex II** data, **will** become available for only **very** few chemicals.

The large number of expected data gaps **creates** the need for estimation methodologies (e.g. Quantitative Structure-Activity **Relationship (QSARs)**). Although the use of estimation methods is a **pragmatic choice**, their limitations should be taken into **consideration** [3]. The present status of **QSAR research** **has** reached the point where these techniques **can** be used, with due **precaution**, for estimation **and prediction** of fate and **effect parameters**. In some cases the **parameters can** be predicted with **such** a high level of reliability that the setting of (preliminary) quality criteria **based** on these **predictions** is justified. In other cases, however, the models are