4.2.2. Ecotoxicity parameters

4.2.2.1. Toxicity to aquatic organisms

For predicting aquatic toxicity approximately 300 SAR models are available to the EPA experts for various (about 100) chemical classes. The estimation methods are mostly based on log P_{ow}; only calculated values of this latter parameter are used. Expert knowledge is required for the selection of the appropriate SAR model. The selection is based on the chemical class, not on the mode of action. The EPA's SAR predictions cover both acute and chronic toxicity for aquatic organisms. Fish, daphnia, algae and, for some pesticid structures, also vascular plants are considered. For some chemical classes, if log P_{ow} is above 5 it is assumed that there are no acute toxic effects. Nevertheless, for those substances, and similarly for chemicals for which no toxic effect is predicted at the water solubility limit, chronic effects may still be substantial. The data on aquatic toxicity are used for risk assessment and assignment of "level of concern".

In the EC according to the requirements of Directive 79/831/EEC (sixth Amendment) at "base set" level, normally only acute fish and daphnia studies are conducted. Chronic effects and effects on species other than fish and daphnia, e.g. algae, are in general not addressed at this stage. The aquatic toxicity data are used for risk assessment and for the classification "dangerous for the environment".

In several cases, the data were given as $>n$, $<n$ or as NTS (Non Toxic at Saturation). LC/EC50 data given as $<n$ are difficult to interpret because in those cases, the actual LC/EC50 value can be much lower than the given limit. For this reason those data were excluded from analysis. Values given as $>n$, however, can be used because usually, the given limit will be regarded as a worst case estimate of the toxicity. The analysis includes therefore those chemicals for which exact and "higher than" ($>n$) effect concentrations are supplied; data presented as NTS are also included.

The comparative analysis is carried out applying the following criteria:

- for all values given as $>n$ the numbers are directly compared without considering the signs;
- for data pairs with both values above 100 mg/l, no differentiation is made between the numerical values: the ratio of estimated/measured value therefore is 1;
- the values are considered to be in agreement if they are within $\pm$ 1 log unit;
- for data pairs in which one value is given as NTS and the other as a numerical value, the results are assessed considering the water solubility: for a numerical value much higher than the water solubility (>100 mg/l) the SAR and experimental value are deemed to be in agreement; for effect concentrations closer to the water solubility (<100 mg/l) the two values are deemed to be inconsistent with one another (disagree).

The results of the comparative analyses are given in Table 6 (Toxicity to fish) and Table 7 (Toxicity to daphnia, the detailed analyses are given in the Annexes 9 and 10.

TABLE 6: Comparison of data on toxicity to fish

	N° of chemicals	%
Total	130	100
Agreement	107	82.3
Disagreement	23	17.7
- Overestimation	14	10.8
- Underestimation	9	6.9

TABLE 7: Comparison of data on toxicity to Daphnia

	N° of chemicals	%
Total	127	100
Agreement	90	70.9
Disagreement	37	29.1
- Overestimation	20	15.7
- Underestimation	17	13.4

Some of the differences in predicted and experimental toxicity can be attributed to nominal instead of measured concentrations, the use of solvents to enhance water solubility and to different test durations (24/48 hr for daphnia). For only 5 chemicals were measured and predicted data on algae toxicity available. In 4 cases, agreement between SAR/MPD data is observed (data: see Annex 11).

- Conclusions

Information on aquatic toxicity is used both for risk assessment and for classification purposes. Overall, SAR predictions of aquatic toxicity are quite good. For fish toxicity the predictions tend to overestimate the toxicity. For daphnia over- and underestimations occurred at about the same rate. Further effort is desirable to explain the cases where the reason for the underestimation (false negative predictions) is not evident. Nevertheless, if used with the required caution, SAR predictions can be very effective in the context of the US notification scheme.

The predictions are considered to represent a very useful future option to support the decision taking process within a stepwise risk assessment scheme for carrying out toxicity tests.