

SCRAM: A Scoring and Ranking System for Persistent, Bioaccumulative, and Toxic Substances for the North American Great Lakes *

Part I: Structure of the Scoring and Ranking System [ESPR 7 (1) 51-61 (2000)]

Part II: Bioaccumulation Potential and Persistence [ESPR 7 (2) 115-121 (2000)]

Part III: Acute and Subchronic or Chronic Toxicity

Part IV: Results from Representative Chemicals, Sensitivity Analysis, and Discriminatory Power

Part II. Bioaccumulation Potential and Persistence

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Abstract. Part I (SNYDER ET AL., 1999a) of this series introduced SCRAM, a chemical scoring and ranking (CSR) system for contaminants of the North American Great Lakes. Here, in Part II, scoring of the bioaccumulation potential and persistence of chemicals is discussed, including acceptable types of data, specific scoring instructions, and the basis for criteria and scores for these categories of the system. Difficulties encountered during the process of determining which types of data adequately represent the properties of interest are discussed. Also, justification is given for an emphasis on scoring on the basis of persistence.

Keywords: Acute toxicity; bioaccumulation; chemical scoring and ranking; chronic toxicity; hazard; North American Great Lakes; persistence; priority pollutants; SCRAM (Chemical Scoring and Ranking Assessment Model); uncertainty; water pollution

1 Introduction

In Part I (SNYDER et al., 1999a) of this series, SCRAM, a chemical scoring and ranking (CSR) system for North American Great Lakes contaminants, was introduced. This system was developed to screen large lists of chemicals to determine which deserve the most immediate attention regarding their potential hazard to the environment. This determination is made on the basis of a limited data set including information on the bioaccumulation potential, persistence, and toxicity of each

chemical. The scoring information is entered into a spreadsheet that calculates the score. This part of the series addresses bioaccumulation potential and persistence of chemicals, properties that together represent the potential for exposure. Types of data that are acceptable for scoring are described, and specific scoring instructions are given. Data selection criteria are also discussed. Scoring for acute toxicity and subchronic or chronic toxicity is discussed in Part III of this series (SNYDER et al., 1999b). A literature review was conducted for 21 representative chemicals to determine whether appropriate data were available, and those chemicals were scored in Part IV (SNYDER et al., 1999c) of this series.

2 Data Selection Criteria for Persistence and Bioaccumulation

Data in peer-reviewed literature generated from studies using standardized guidelines or from Good Laboratory Practices (GLP)-certified laboratories are acceptable for scoring in SCRAM. Data from peer-reviewed literature compilations (e.g., HOWARD, 1989a, 1989b, 1989c, 1989d; MACKAY et al., 1992a, 1992b, 1992c; U.S. EPA 1979a, 1979b, 1982) were used to score chemicals if the compilations included a description of data quality so that studies could be judged for acceptability.

3 Bioaccumulation

3.1 Acceptable types of data and specific scoring instructions

Bioaccumulation is the net accumulation of a chemical by an organism via all of the routes of exposure, including up-

* The scoring and ranking system in the form of a Lotus 123⁹⁷ spreadsheet and a description of its use are available on the Internet at <http://www.epa.gov/toxteam/pbtrep/>

take from the environment or ingestion of food or water (SUTER, 1993). In SCRAM the bioaccumulation factor (BAF) is used to produce a score for bioaccumulation so that all routes of exposure are considered in generating the score. A BAF is a ratio of chemical residue in the tissue of test organisms to chemical concentration in an external environmental phase, including water, sediment, and food, at steady state (RAND, 1995). However, a bioconcentration factor (BCF) or an octanol-water partition coefficient (K_{ow}) is more often available in the literature. Bioconcentration is the net accumulation of a chemical directly from an aqueous solution by an aquatic organism (SUTER, 1993). If it is suspected that a chemical will bioconcentrate, it may be subjected to one or more bioconcentration tests which are designed to determine or predict the BCF. The BCF is the ratio of the concentration of test chemical accumulated in the tissue of test organisms under steady-state conditions to the average measured concentration in the water to which the organisms were exposed (RAND, 1995). The BCF does not take into account uptake of a chemical from food, sediment, etc. A K_{ow} is measured by liquid-liquid partitioning of a chemical between octanol and water. The K_{ow} is the ratio, at equilibrium, of the concentration of the chemical in octanol to the concentration in water (RAND, 1995). Sometimes values for the BAF or BCF are estimated from quantitative structure-activity relationship (QSAR) models. All of these are acceptable data, but the order of preference is as follows: measured BAF, measured BCF, K_{ow} , QSAR-estimated BAF, QSAR-estimated BCF. The associated uncertainty scores are, respectively, 0, 1, 2, 4, and 5.

Benthic invertebrates may bioaccumulate toxic substances by ingestion of contaminated sediment or, in the case of substances that partition between dissolved and particle-associated phases, by uptake across portions of the body other than the gut (PENRY, 1998). Various factors affecting ingestion, uptake, and assimilation of toxicants are discussed by PENRY (1998). Uptake of toxicants in fish also might occur via ingestion of food and/or across the gills, and various environmental factors affect these processes (see RAND, 1995).

Appropriate bioconcentration studies should report chemical concentrations in ambient water and in tissue. It is best if test water is analyzed to determine the measured concentrations rather than relying on the nominal concentrations. Some researchers report only a BAF or BCF, and in this case best professional judgment must be used to determine whether the study meets basic experimental quality standards. Whole organism (whole body) tissue concentrations usually are required. In some cases, fish muscle tissue concentrations may be acceptable for scoring metals. Wet weight-based BCFs are used for scoring because these are most often available in the literature. Lipid-adjusted BCFs can be converted to weight-based BCFs if the average lipid composition of the test species is known (as is often true for fish) or if the measured lipid composition is reported with the BCF data. Data from studies using flow-through exposure systems with either continuous or intermittent flow are preferred. However, data from static exposure studies might be used in some cases for short-term tests with chemicals

that are stable in the exposure system. Test chemical concentrations should be great enough to permit detection in tissue and water samples but small enough to remain below the limit of solubility (FRANKE, 1996; RAND, 1995). Because use of solubilizers to dissolve hydrophobic substances at concentrations above their true water solubility can result in underestimation of BCF values, scoring on the basis of tests using such methods should be avoided (FRANKE, 1996). Test concentrations should fall within those that reasonably could be expected in the environment.

$\log K_{ow}$ is used for scoring because it is often correlates well with BCF data through log-log correlations for organic chemicals to which organisms are exposed mainly through water. These correlations do not work well for contaminants that are quickly biotransformed. Also, for chemicals that are "superhydrophobic," i.e., those with $\log K_{ow}$ greater than 6, these correlations can lead to an overestimate of the BCF. This may be due to decreased bioavailability of the chemical because of sorption to organic phases in the environment or to decreased permeability of biological membranes to these chemicals relative to those with lesser hydrophobicity (RAND, 1995). For example, gill uptake efficiency for chemicals with $\log K_{ow}$ greater than 6.5 tends to decrease with increasing $\log K_{ow}$. Different theories have been used to explain this phenomenon. It might be due to increasing binding of chemical to dissolved organic carbon in the water. Another explanation is that larger molecules might be taken up more slowly because of molecular size and decreased diffusion across gill epithelium (BURKHARD, 1998). In this case, using greater $\log K_{ow}$ values to predict greater bioconcentration leads to a conservative estimate of bioconcentration potential for superhydrophobic chemicals, so it is not a serious concern for a screening activity. Professional judgment can be used at this step to determine whether the maximum score is deserved for superhydrophobic chemicals. Conversely, bioconcentration of hydrophilic chemicals ($\log K_{ow}$ less than 1) might be underestimated by use of the $\log K_{ow}$. An example of an important contaminant for which $\log K_{ow}$ does not predict bioconcentration or bioaccumulation is methyl mercury. Even though it has a relatively low $\log K_{ow}$ of 2, it accumulates in aquatic organisms by binding to sulfhydryl groups on proteins. Liquid-liquid partitioning will not predict this binding. Therefore, special attention should be given to hydrophilic chemicals to determine whether this type of accumulation may occur.

$\log K_{ow}$ is not always a good predictor of bioaccumulation potential. For example, FISK et al. (1998) examined dietary accumulation data for 23 hydrophobic organochlorines (OCs) administered to juvenile rainbow trout. They found that the \log BMF for OCs with $\log K_{ow}$ less than 7 increased with increasing $\log K_{ow}$, but \log BMF decreased with increasing $\log K_{ow}$ for OCs with $\log K_{ow}$ greater than 7. This is similar to the pattern observed for the relationship between \log BCF and $\log K_{ow}$. Therefore, OCs with $\log K_{ow}$ of approximately 7, and which are not biotransformed, had the greatest potential to biomagnify and persist in these fish (FISK et al., 1998). The authors of the study offer a possible explanation for the curvilinear relationship between $\log K_{ow}$ and \log BMF (FISK et al., 1998). Moderately

hydrophobic chemicals might reach slower clearing compartments within the fish more quickly than superhydrophobic chemicals do. The moderately hydrophobic chemicals may take longer to clear from the fish during the depuration phase of the test because they have reached slower clearing compartments in greater proportions. Because of this curvilinear relationship, a superhydrophobic chemical might receive an undeserved high score for bioaccumulation if the score is based on $\log K_{ow}$. However, again, this results in a conservative score for superhydrophobic chemicals that can be altered according to the user's professional judgment during the scoring and ranking activity or during a subsequent risk assessment.

There are various reasons for imposition of a greater uncertainty score for $\log K_{ow}$ data than for measured BAF or BCF data. In addition to the fact that $\log K_{ow}$ is not always a good predictor of BAF or BCF, there can be a significant degree of variation in measurement or prediction of $\log K_{ow}$ itself, depending on the method used and the type of chemical tested. Hydrophobic chemicals can pose special experimental problems such as formation of micelles and emulsions in the aqueous phase during liquid-liquid partitioning, leading to more variable results (BURKHARD, 1998). However, the variability in the result depends on the method used. The slow-stir technique generally yields less variable results for hydrophobic chemicals (BURKHARD, 1998). Assignment of even greater uncertainty scores for estimated BAF or BCF data relative to measured BAF, measured BCF, or $\log K_{ow}$ values is justified by the fact that these estimated data are often based on $\log K_{ow}$ and other data that have their own intrinsic variability. This variability can be magnified or reduced by models (BURKHARD, 1998).

For some chemicals, more than one value useful for scoring can be found in the literature. In that case, after all acceptable data have been gathered, the data points are separated according to the class of organism tested (e.g., fish, mollusks, *Daphnia*), and the geometric mean of all values for data of the greatest preference (e.g., $BAF > BCF > K_{ow}$) within a class is used to calculate a class-mean. The geometric mean of the class means is used to assign a bioaccumulation chemical score. Then the number of uncertainty points associated with the data type used is entered into the spreadsheet.

3.2 Basis for criteria and scores

Criteria and metrics for this scoring system were determined after reviewing existing scoring systems. SCRAM uses BAF, BCF, K_{ow} , QSAR-estimated BAF, and QSAR-estimated BCF values to rank the bioaccumulation potential of chemicals. The system uses five tiers of values, ranging from a minimum value of <100 to a maximum of >100,000. The Michigan Critical Materials Register (CMR) uses the same metrics and accepts BAF, BCF, or $\log K_{ow}$ values but also uses an asterisk designation to indicate "insufficient evidence" to score the chemical for bioaccumulation (MDNR, 1987). SCRAM uses a numerical score instead to indicate the level of uncertainty associated with the score given. The general trend for most other scoring systems that were reviewed was use of a smaller range of BCF, BAF, K_{ow} , or water solubility values to score bioaccumulation, with a maximum value less

than that used in SCRAM. Some scoring systems use only a trigger value above which a chemical is considered to be bioaccumulative and below which it is not.

3.3 Specific conditions, concerns, and biases

There are some important factors that should be considered when selecting bioaccumulation data for lipophilic substances in fish. $\log K_{ow}$ often does not predict BCF or BAF very well for chemicals that are readily transformed. Different life stages of fish have different metabolic capacities that can affect the determination of bioaccumulation or bioconcentration potential. For example, in a study conducted with a series of lipophilic chemicals on different life stages of fish, it was determined that body burdens of chemicals readily transformed by juvenile and adult fish may accumulate to a greater degree in early life stages due to their lesser metabolic capability (PETERSEN and KRISTENSEN, 1998). In addition, early life stages tend to have greater lipid content and greater surface area (total body and gill) to weight ratio than juvenile and adult fish, and this can cause differences in accumulation of lipophilic chemicals (PETERSEN and KRISTENSEN, 1998). Lower exposure temperatures also can result in a slower rate of metabolism of test compound and alter the results of bioaccumulation or bioconcentration tests (PETERSEN and KRISTENSEN, 1998).

4 Persistence

4.1 Acceptable types of data and specific scoring instructions

One of the distinguishing features of SCRAM is the emphasis placed on using persistence to score and rank chemicals. Acute toxicity data (especially lethality data) typically are more readily available than are chronic toxicity data. Thus, chemicals that are not very persistent and bioaccumulative but that are acutely toxic are likely to draw notice simply because of their acute toxicity. However, it is possible that adverse effects other than acute toxicity will not be recognized immediately because the effects are subtle or because they have not been investigated. Chemicals that are persistent in the environment are more likely to bioaccumulate and/or cause chronic effects that may be missed. For these reasons, lack of data regarding chemical persistence results in a greater number of uncertainty points than does lack of data in other categories. Both bioaccumulation and persistence in biota are scored, even though the two types of data are somewhat similar. Use of both types of data is a part of the emphasis on using persistence to score chemicals, a bias that was intentionally incorporated into the design of the system. Continuous environmental inputs of a chemical might also increase exposure, but a satisfactory method for dealing with environmental inputs has not been developed yet for SCRAM.

Because a chemical half-life is required for each of five environmental compartments (biota, air, soil, sediment, and water), SCRAM considers a chemical that has left a particular compartment to be gone for the purposes of that compartment. For example, a half-life for vaporization from soil can be used as a half-life in the soil compartment. The chemi-

cal has not disappeared from the environment (i.e., it has not been degraded to some other chemical), but it has disappeared from that compartment. Its presence in another compartment to which it has moved presumably will be identified as the user fills in the values for persistence in the other compartments. The user should be aware that it is possible that the persistence score could be artificially low in the special case that transfer rates among environmental compartments are great and no environmental sink exists.

Other types of data are acceptable in addition to a half-time to degradation, but only if the data used represent a major route of removal (→ *Table 1*). For example, if data in the literature indicate that the hydrolysis half-life for a chemical in air will be slow (on the scale of years) and the photolysis half-life in air is 3 days, the photolysis half-life should be used for scoring because the other is not a major route of removal of the chemical from that compartment. Multi-media models (discussed below) can aid in determining which are the most likely sinks and routes of removal for a chemical in the environment so that decisions can be made about which specific routes of removal are most important or appropriate for scoring. Another risk ranking system developed for the European Union (EURAM, or EU Risk Ranking Method) uses a Mackay level I model to assess distribution of a chemical emission into different environmental compartments during its ranking process (HANSEN et al., 1999). Other types of data not listed in *Table 1* might be deemed useful and acceptable for the user's purposes.

Table 1: Some acceptable persistence data types for each of the five environmental compartments

<i>Air</i>	<ul style="list-style-type: none"> • hydrolysis half-life in air • photolysis half-life • half-life for reaction with singlet oxygen, hydroxyl radical, alkylperoxy radicals, ozone, or nitrate radical • half-life for volatilization from water
<i>Water</i>	<ul style="list-style-type: none"> • hydrolysis half-life • photolysis half-life in water • half-life for biodegradation in water • half-life for volatilization from water
<i>Soil</i>	<ul style="list-style-type: none"> • half-life for volatilization from soil • half-life for biodegradation in soil • half-life for leaching from soil into a body of water
<i>Sediment</i>	<ul style="list-style-type: none"> • half-life for biodegradation in sediment
<i>Biota</i>	<ul style="list-style-type: none"> • half-life for depuration • half-life for metabolism

Biodegradation is "any process mediated by living organisms that results in the conversion of an organic chemical into organic and/or inorganic end products which are chemically distinct from the parent material" (LARSON and COWAN, 1995). Bacteria and fungi are primarily responsible for the occurrence of this process in the environment. Mineralization, or complete degradation to carbon dioxide or methane, is the preferred end point for scoring. However, the chemical of interest might be degraded to toxic and/or persistent metabolites.

If it is known that degradation products of a chemical are responsible for all or most of its toxic effects, the degradation products should be scored as well, and the results for the degradation products should be reported with the results for the parent chemical. A biodegradation test that conservatively measures the potential of a chemical to persist and/or form persistent intermediates is the carbon dioxide evolution test. The test system is dosed with the chemical of interest, which serves as a sole carbon source, and carbon dioxide production is measured (LARSON and COWAN, 1995).

In the biota compartment, both metabolism and depuration may be considered. Metabolism data should be used with caution and considered only if the chemical is transformed to a harmless form or its transformation results in clearance of the chemical from the organism. For some chemicals, metabolism within the organism is required to produce toxic effects or the chemical is metabolized to another that is still toxic. If this is the case, the chemical cannot be considered cleared from the organism until these toxic metabolites are also cleared. In the case where a chemical is transformed to a form deemed to be harmless, it should be considered that it might be causing toxic effects that simply have not been observed (e.g., the metabolite might be acting through an unanticipated mechanism).

A measured compartment half-life is preferred over half-lives for specific routes of removal.

Sorption is not included in the list of acceptable types of data because a chemical adsorbed to particulate matter in water, for example, is not really removed from the water. Although it is not available for some other processes at the time that it is adsorbed to particulates, it could desorb and become available again. Resuspension from sediment or deposition rates from air would be difficult to score, since it is unlikely that one will find a half-life value in the literature to describe these processes. Measured half-life values are preferred for scoring, but if a value is not available for a particular compartment, a multi-media model may be used to estimate the half-life. Examples of multi-media models that may be used are the Mackay fugacity model (MACKAY and PATERSON, 1991), Simple Box (LAKE et al., 1987), and the Gobas trophic level model (GOBAS et al., 1988). Volatilization from water and photolysis in water are restricted to the first few meters of depth. All elemental chemicals are considered to be persistent because they are always present in the environment. Non-radioactive elements automatically receive a persistence chemical score of five and a persistence uncertainty score of zero.

Certain types of data are not suitable for scoring chemical persistence in SCRAM. Some chemical degradation tests are carried out in solvents other than water and are not intended to simulate environmental conditions. Some volatilization tests are conducted under conditions not comparable to environmental conditions. Such studies do not generate results that adequately represent chemical behavior in the environment. Only environmentally relevant data should be used for scoring in SCRAM.

If more than one half-life value is found for any single compartment, the geometric mean of the data of greatest prefer-

ence should be used to score that compartment. Taking the geometric mean tends to reduce the effect on the score of one value that is radically different than the others. When the authors examined, for example, a list of BCF values or log K_{ow} values for the same chemical, it was not uncommon for most of the values to be clustered close together, with one or two significantly different from the rest. The geometric mean was used for fate data (i.e., persistence and bioaccumulation) because these data can vary to a great extent depending on the type of test run and the environmental or laboratory conditions occurring at the time of testing. Because the goal is to derive environmental fate scores applicable to general environmental conditions, the geometric mean was used instead of the most restrictive value. However, the user might decide to use the most restrictive value if that suits the purpose of the scoring activity. The most restrictive value is used to score toxicity because the goal is to protect plant and animal life, and it is likely that there are more sensitive species in the environment than those for which there were toxicity data available. Toxicity scoring is discussed further in Part III of this series (SNYDER et al., 1999b).

4.2 Basis for criteria and scores

Criteria and metrics for this scoring system were determined after reviewing numerous existing scoring systems. The scoring systems reviewed dealt with persistence in many and varied ways, including avoidance of the subject, narrative descriptions, and numerical scoring. Even among the numerical scoring systems, the number and range of scores varied. SCRAM uses half-life data for each of five environmental compartments (biota, air, soil, water, and sediment) to score persistence.

The metrics are the same for each compartment, with half-life values ranging over five scoring tiers, from a minimum of <4 days to a maximum of >100 days. Candidate Substances for Bans, Phase-outs or Reductions-Multimedia Revision from the Ontario Ministry of the Environment Scoring System (OMOEE, 1993) uses four scores ranging from zero to ten for half-lives from less than or equal to ten days to greater than 100 days. The Chemical Scoring System for Hazard and Exposure Identification (O'BRYAN and ROSS, 1988) uses five scoring categories with scores from one to five for half-lives ranging from less than one day to greater than one year. The CMR (MDNR, 1987) uses three scoring categories with different scoring tiers for hydrolysis and evaporation, and uses an asterisk designation to indicate "insufficient information" to score the chemical. Elements of these and other scoring systems were used to design the one currently used for environmental persistence in SCRAM.

4.3 Specific conditions, concerns, and biases

The scoring category for persistence was particularly difficult to develop. Others who have designed chemical scoring and ranking (CSR) systems also had difficulty dealing with persistence data. This is due in part to the lack of a good working definition of persistence. Another contributing factor is the difficulty in determining what types of data adequately represent the persistence of a chemical, especially since persistence varies by environmental compartment. Scarcity of peer-reviewed data related to persistence plagued ef-

forts to address those issues. Actual measured environmental concentrations of chemicals are difficult to find. Factors including seasonal variations in temperature and precipitation add to the variability of chemical concentrations in a single site over time, so that a single measurement may not be representative of year-round concentrations. Soil type, climate, topography, and ground cover can affect persistence of a chemical in the environment, so that measurements of a chemical in one site might give little indication of the levels that could be expected in another site receiving similar chemical releases. Particularly difficult to find were half-lives for persistence in sediment and soil.

Although results from laboratory studies are available more frequently than are measured environmental values, the results of laboratory studies are often difficult to relate to chemical behavior in the environment. It is challenging to make predictions that are both general enough and realistic enough to be useful. Despite the difficulty of dealing with persistence in this context, this system makes use of the more reliable types of persistence data. Future improvements in scoring chemicals should involve better tests of persistence and methods of incorporating this information into scoring systems. Currently, the best option is to couple level III multi-media models with scoring systems. The level III spreadsheet multi-media model is similar to the scoring system in that it provides a template with which to frame issues and a listing of the information required to describe the environmental fate profile of a chemical.

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Environmental Protection – ACHEMA 2000 Faces New Challenges

From 22 to 27 May 2000, the exhibition grounds in Frankfurt am Main will host ACHEMA 2000 - the world's most important Exhibition Congress and International Meeting on Chemical Engineering, Environmental Protection and Biotechnology.

With more than 4,000 exhibitors from 47 countries, ACHEMA 2000 will again set a string of new records. Around 1,500 exhibitors from all exhibition groups will present the latest processes, plants, apparatus and services for all areas of environmental protection like air pollution control, water and waste-water treatment, waste technology and recycling, soil remediation, noise abatement, environmental measurement techniques and analysis, energy conservation and material flow, and energy management.

Production-integrated environmental protection aims to minimise the flow of environmentally relevant substances, the consumption of resources as well as costs. Visitors to the ACHEMA will find state-of-the-art equipment which offers solutions that meet the demands of both production and environment. Examples:

- Catalysts for higher chemical conversion with increased energy efficiency

- separation and isolation techniques for recovering products and auxiliary substances from gaseous, liquid and solid media
- reprocessing and recycling methods for wastes and residues
- energy-saving thermal processes and technologies for energy recovery
- measurement techniques and sensors for optimum process management
- new approaches for production-integrated environmental protection by biotechnology

Comprehensive congress programme for environmental protection
 The ACHEMA 2000 International Congress will present more than 200 lectures on the latest developments in research and industry for environmental protection. Up-to-date information is available via Internet www.achema.de.

Exhibitors, lecturers and the organizer of the event are already looking forward to greeting international specialists in Frankfurt am Main in May and wish you all an eventful, informative, innovative and stimulating visit to ACHEMA 2000.

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