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A Relative Risk Ranking of Pesticides Used in Prince Edward Island

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Environmental Protection Branch
Atlantic Region
Environment Canada
5th Floor, Queen Square
45 Alderney Drive
Dartmouth, Nova Scotia
B2Y 2N6

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A Relative Risk Ranking of Pesticides Used in Prince Edward Island

Allison M. Dunn

Environmental Protection Branch
Environment Canada
Atlantic Region

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ABSTRACT

Establishing priorities for regulatory and scientific assessments of pesticides is difficult given the large number of registered pesticide products and varied use patterns of each product. According to the general paradigm of "Risk = Toxicity x Exposure", a relative risk ranking of agricultural pesticides was developed using a modified Chemical Hazard and Evaluation for Management Strategies (CHEMS) model. Release-weighting factors were derived using pesticide sales information. Factors for each active in each media were determined on a scale of 1 to 10 relative to the largest pesticide release in each respective media. A risk score was then tabulated by multiplying the sum of release-weighted toxicity endpoints (*i.e.* acute oral LD_{50}, acute inhalation LC_{50}, carcinogenicity rating, no observed adverse affect level, acute fish LC_{50}, acute *Daphnia* EC_{50}) by the sum of weighted exposure factors (*i.e.* soil half-life, log BCF). While the model makes use of toxicity and exposure data, the risk ranking produced does not represent a risk assessment. Rather, the results from CHEMS should be viewed as a quantitative risk ranking used to prioritize substances for future risk assessment and management activities. Hazard and exposure data were collected for a subset of 31 active ingredients, representing 94% of Prince Edward Island's 2001 pesticide sales by mass. According to the resultant risk scores, the highest ranked substances were chlorothalonil, diquat dibromide, mancozeb, metiram, and carbofuran. Limitations included the use of pesticide sales data as a proxy for release and the reliance on modelled data for log BCF and determining environmental partitioning. In spite of its limitations, the CHEMS risk ranking scheme provides a useful tool for prioritizing pesticides of concern for future action.

RÉSUMÉ

Établir des priorités pour des évaluations réglementaires et scientifiques des pesticides est difficile étant donné le grand nombre de produits pesticides et schémas d'usage variés de chaque produit. Selon le paradigme général du 'Risque = Toxicité x Exposition', un classement relatif du risque des pesticides agricoles était développé en employant un modèle modifié du Chemical Hazard and Evaluation for Management Strategies (CHEMS). Des facteurs de rejet étaient dérivés en employant de l'information sur la vente des pesticides. Des facteurs pour chaque matière active dans chaque média ont été déterminés par une échelle de 1-10 relatif à la plus grande rejet dans chaque média respectif. Une note de risque était ensuite calculée en multipliant la somme des valeurs de toxicités pesées (*i.e.* de la toxicité orale aiguë, de la toxicité aiguë par inhalation, l'évaluation des carcinogènes, la dose sans effet observable, de la toxicité de poisson aiguë, *Daphnia* sp., toxicité aiguë) par la somme des facteurs d'exposition pesée (*i.e.* la demie vie du sol, la BCF). Alors que le modèle utilise les données de la toxicité et l'exposition, le classement de risque résultant ne représente pas une évaluation de risque. Plutôt, les résultats du CHEMS devraient être vus comme classification qualitative et l'interprétation la plus appropriée est de considérer des groupes chimiques. Des données du hasard et de l'exposition étaient cueillies pour un sous-ensemble de 31 ingrédients actifs, représentant 94% des ventes des pesticides à l'Île-du-Prince-Edouard en 2001. Selon les notes du risque résultants, les substances de la plus haute note incluaient le chlorothalonil, le diquat dibromide, le mancozeb, le metiram, ainsi que le carbofuran. Les limites incluaient l'usage des données de ventes des pesticides comme substitut pour les rejets et la dépendance de données modelées pour la BCF et pour déterminer le budget environnemental pour chaque actif. Malgré ses limites, le schéma de classement de risque CHEMS fournit un outil utile pour donner la priorité les pesticides d'inquiétude pour une action future.

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1.0 INTRODUCTION

In 2001, more than 800 tonnes of active ingredients were purchased by Prince Edward Island's (PEI) agricultural community. Given its extensive potato growing area and the high reliance of that crop on pesticide use, PEI is one of the more intensive users of pesticides in the country. Pesticides have been linked to sporadic fish kills in PEI following rain events (Mutch *et al.* 2000, InfoPEI 2004).. In addition to environmental impacts, regulators of PEI's agricultural community are also concerned with the possible link between pesticides and adverse health effects. Such concerns are not unfounded considering the abundance of pesticide-based ecological and health studies undertaken by the scientific community over the last 50 years (Ritter 1997).

Given the widespread use of pesticides in PEI and their possible link to adverse environmental and health outcomes, there is interest in developing a priority listing of pesticides to help direct and prioritize future risk assessments and risk management activities with respect to pesticides. Previous work undertaken by PEI's Department of Technology and Environment (Mutch 1999) provided a relative ranking of the acute pesticide risks to fish by dividing a pesticide's application rate by its respective rainbow trout LC_{50}. While this method provided a rough estimate of the acute aquatic risks posed by pesticides in PEI, a model that included the other underlying factors influencing a pesticide's risk (e.g. environmental fate, health effects) would be much broader in application and more precise in estimating risk.

To this end, the CHEMS risk ranking model, developed by the University of Tennessee's Center for Clean Products and Clean Technologies, is an example of an algorithm which includes human health, environmental and exposure endpoints to yield a relative risk ranking for a group of chemicals (Swanson *et al.* 1997). The model has been used to generate a relative risk ranking for the U.S. Toxic Release Inventory (TRI) which includes both pesticides and industrial chemicals (Swanson *et al.* 1997). Further, the model has also been used by Environment Canada's Atlantic region to yield a relative risk ranking of the 1999 National Pollutant Release Inventory (Environment Canada 2000).

Environment Canada, Atlantic Region recently applied a modified version of the CHEMS model to high volume pesticides used in PEI. The outcome of this exercise, including an overview of the model, a description of the data collection procedure, data treatment, and the model's limitations and uncertainties are provided in the body of this report.

2.0 MODEL OVERVIEW

The CHEMS model combines hazard and exposure endpoints to yield a relative risk ranking for a group of substances. Following the general paradigm of "Risk = Toxicity x Exposure", a risk score is tabulated by multiplying the sum of weighted toxicity endpoints by the sum of weighted exposure endpoints:

Risk Score = [sum of weighted toxicity endpoints] x [sum of weighted exposure endpoints]

When risk scores have been tallied for all substances in a group, the substances can be ranked accordingly. Presumably, the higher ranked substances will pose a higher risk, while lower ranked substances will present a lower risk to the environment. Although the model makes use of measured and estimated toxicity and physical/chemical endpoints, the CHEMS risk ranking scheme does not represent a risk assessment and should not be construed as such. Rather, the resultant quantitative risk ranking can be best used to identify relative groupings of high, medium and low risk substances. While any risk assessment method has limitations, the CHEMS approach attempts to provide an intermediate solution along the risk assessment continuum.

2.1 Selection of Active Ingredients for Risk-Ranking

To expedite and make more efficient the data gathering process, active ingredients purchased at greater than 1000 kg in 2001 were targeted. Based on this criterion, the final data set included 31 active ingredients which comprised 94% of the mass of PEI's pesticide sales for 2001.

2.2 Toxicity and Fate Measures

The modified CHEMS model employed by Environment Canada used six toxicity and three fate parameters to measure the overall hazard of a substance. Table 1 illustrates the toxicity parameters used to represent human health and environmental effects. Bioaccumulation, persistence and release amounts were included to represent a substance's exposure potential.

Table 1: Parameters used by modified CHEMS model to represent exposure potential, human health and environmental effects

EFFECT / Parameter	Endpoint	Definition
HUMAN HEALTH		
Acute Oral	Rat Oral LD_{50}	The quantity of a substance, expressed as the mass of substance per mass of test animal (mg/kg), which causes 50% mortality in a group of test animals within 14 days given a single oral dose.
Acute Inhalation	Rat Inhalation LC_{50}	The concentration of a substance in air, expressed in mg/L, which causes 50% mortality in a group of test animals when inhaled continuously for 4 hours.
Chronic	Carcinogenicity	Based on United States Environmental Protection Agency (US EPA) and International Agency for Research on Cancer (IARC) classifications.
Chronic	Non-carcinogenic	Based on the most sensitive specie's oral no-observable adverse effect level (NOAEL). The NOAEL represents the highest test concentration that does not show any deleterious effects in the test animals.

EFFECT / Parameter	Endpoint	Definition
ENVIRONMENTAL		
Acute aquatic	Fish 96-hour LC_{50}	The concentration of a substance in water (mg/L) which causes 50% mortality in a group of test fish (*Onchorrynchus mykiss*-rainbow trout) exposed continuously for 96 hours.
Acute aquatic	Water Flea 48-hour LC/EC_{50}	The concentration of a substance in water (mg/L) which causes 50% mortality or immobilization in a group of test animals (*Daphnia magna*) exposed continuously for 48 hours.
EXPOSURE POTENTIAL		
Persistence	Soil Half-life	Soil half-life is the time required for a substance to biodegrade to half its original concentration in a soil lab test under aerobic conditions and in the presence of mixed populations of micro-organisms. When study conditions were described, studies conducted with sandy loam were chosen since this soil type is representative of agricultural soils in PEI. In the absence of soil half-life data, the field dissipation half-life was used. The field dissipation half-life is the time required for a substance to dissipate to half its original concentration under field conditions.
Bioaccumulation	Aquatic Bioconcentration Factor (BCF)	The ratio of the concentration of the chemical in an aquatic organism to that in water at steady-state. When measured data were not available, this parameter was estimated using a quantitative structure-activity relationship (QSAR).
Release Amount	Release Weighting Factor (RWF)	Calculated using the quantity of active ingredient distributed among various media (air, water, land). Environmental partitioning of active ingredient determined by Level III Fugacity multi-media model provided by US EPA's EPI Suite v3.10.[a]

[a] EPI Suite v3.10 is a collection of quantitative structure-activity relationship (QSAR)-based software that provides estimates for a number of environmental fate properties.

3.0 DATA SOURCES AND TREATMENT

A considerable effort was made to collect data from reputable sources. While an abundance of pesticide-related sources are available, only a few select references and websites were consulted for pesticide data as described below.

3.1 Human Health Effects Data

The majority of human health toxicity data were obtained from monographs provided by the Joint Meeting on Pesticide Residues (JMPR), US EPA's Integrated Risk Information System (IRIS), International Agency for Research on Cancer (IARC), the US EPA's Re-registration Eligibility Decision (RED) documents, supporting documentation for the EPA REDs or the British Crop Protection Council's Pesticide Manual (Tomlin 2000). On occasion, when information was lacking for an active ingredient from these sources, monographs provided by the International Programme on Chemical Safety [e.g. Environmental Health Criteria Monographs, Joint Expert Committee on Food Additives (JECFA)] and the Hazardous Substances Data Bank (HSDB) were consulted.

Acute rat oral LD_{50} values and inhalation LC_{50} values were primarily obtained from the Pesticide Manual and monographs provided by JMPR, REDs or documents supporting REDs. When more than one toxicity value was obtained for an active ingredient, the geometric mean was taken of all the values. The geometric mean, rather than the arithmetic mean, was used for all toxicity endpoints since the distribution of sensitivities of individual organisms in toxicity tests on most materials are more likely to be log normal than normal (Federal Register 1995). Before calculating the geometric mean, a careful inspection of the upper and lower confidence limits of each LD/LC_{50} was made to ensure that duplicate values were not included in the average.

Carcinogenicity ratings or supporting information on which to base carcinogenicity ratings were obtained from IARC, RED, JMPR, IRIS or Canada's Pesticide Management Regulatory Agency (PMRA). When a carcinogenicity rating was not specified implicitly by any of the cited sources, expert judgement was used to assign a rating following the principles outlined by IARC and the EPA.

The NOAEL for each active was obtained from a number of sources, including REDs, JMPR, IRIS, and the Pesticide Manual. An effort was made to select the NOAEL in which a Reference Dose (RfD) or Acceptable Daily Intake (ADI) was based. The RfD or ADI is the lifetime, average daily dose of a substance an individual can be exposed to without suffering adverse affects. When different conclusions were made by different authorities with respect to RfDs or ADIs, expert judgement was used to select the most appropriate study for establishing the NOAEL. When determining an ADI or RfD, the selected NOAEL is usually divided by an uncertainty factor of 100 (10 to account for interspecies extrapolation and 10 for intraspecies variability). In some cases, where the toxicological database for a substance is incomplete, a NOAEL is not established, a sub-chronic test is used to establish the NOAEL, or there appears to be increased sensitivity to the young, an additional safety factor ranging from 1 to 10 is applied to account for this uncertainty. When an additional uncertainty factor, beyond the standard 100, was recommended by an authority or warranted by expert judgement, the NOAEL for a pesticide was divided by the recommended additional uncertainty factor to permit a consistent comparison of NOAEL values across pesticides. This adjusted NOAEL was used to represent the NOAEL in the modified CHEMS model.

3.2 Environmental Effects Data

Acute aquatic data were sourced from the US EPA's ECOTOX Database and the Pesticide Manual. Again, when more than one value was obtained for an active ingredient, the geometric mean was calculated. Before calculating the geometric mean, a careful inspection of the upper and lower confidence limits of each EC/LC_{50} was made to ensure that duplicate values were not included in the average. Studies conducted with formulated products and active ingredients were both included in the geometric mean. Concerns regarding this practice are negated since the toxicity values from formulated products were adjusted to reflect the percent concentration of active ingredient in the product. While toxicity tests conducted with the active ingredient are preferred, these studies were scarce and in many cases the concentration type was not specified.

However, for the pesticides under investigation, when a toxicity value was available for the active ingredient, it generally was either greater than or within the same magnitude of the geometric mean determined for the pesticide using both formulated and active ingredient studies. Therefore, using the geometric mean over toxicity values derived from the active ingredient was more conservative in some cases.

The original CHEMS model included a chronic aquatic endpoint (*i.e.* fish NOEC). However, since fish NOECs were not readily available in the literature and the QSAR suggested by the model for estimating fish NOECs was a permutation of other data used in CHEMS (*i.e.* log K_{ow} and 96-hour fish LC_{50}), the NOEC was not perceived to add value to the model and was excluded. For example, in the CHEMS risk ranking of the TRI, all of the fish NOEC values were estimated using a QSAR based on 96-hour fish LC_{50} and log K_{ow}. The original CHEMS model also included an acute terrestrial parameter represented by the rat oral LD_{50} under environmental effects. However, by including this endpoint twice in the model, the rat oral LD_{50} was doubly weighted. For our purposes, this endpoint was removed and a new environmental effect parameter was added to the model (*i.e. Daphnia magna* LC/EC_{50}). Other environmental endpoints were explored for inclusion in the model, however, due do lack of available, consistent data, *Daphnia magna* LC/EC_{50} was the only suitable endpoint that could be added to CHEMS.

3.3 Exposure Potential Data

The majority of fate data were sourced from the Pesticide Manual, the Physical-Chemical and Environmental Fate Handbook (Mackay *et al.* 2000), or the US Department of Agriculture (USDA) Pesticide Properties Database. In the original CHEMS model, persistence was represented by water half-life determined by taking one over the sum of inverse function of a substance's biological oxygen demand (BOD) half-life[1] and the inverse function of a substance's hydrolysis half-life:

$$Water\ Half-life = \frac{1}{\left(\frac{1}{BOD} + \frac{1}{Hydrolysis}\right)}$$

However, after conducting a thorough literature search, it was determined that BOD half-lives were not readily available in the literature. Consequently, BOD was replaced with soil half-life. This modification seemed reasonable because soil is the most relevant environmental medium for the pesticides under investigation. Upon further inspection of the water half-life equation, it was decided to base persistence on soil half-life alone. Since the faster fate process is the predominant factor determining water half-life, it is possible that an active ingredient with a quick hydrolysis rate could appear to have a much smaller environmental persistence than predicted by soil half-life. Therefore, to add a level of conservatism to this parameter, soil half-life alone was chosen to reflect

[1] BOD half-life is the time required to biodegrade a chemical such that its BOD in water is reduced by 50%.

persistence. In addition, since soil contains pore water, presumably hydrolysis is already accounted for in the soil half-life.

Bioconcentration factors for whole fish and edible portions of fish were obtained from Mackay's Handbook or the US EPA REDs. Although bluegill sunfish (*Lepomis macrochirus*) is the preferred species for this measure, bioconcentration factors from different fish species were included due to scarcity of bioconcentration data. When more than one measured value was available, the arithmetic mean was calculated. If measured values were not available from the above sources, the bioconcentration factor was estimated by the following QSAR developed by Bintein *et al.* (1993):

$$\log BCF = 0.910(\log K_{ow}) - 1.975 \log[(6.8 \times 10^{-7})K_{ow} + 1] - 0.786$$

Log K_{ow} values used in the QSAR were sourced from the Pesticide Manual or Mackay's Handbook. Again, when more than one measured value was available, the arithmetic mean was calculated.

Determination of the release weighting factors will be discussed later in the report.

4.0 HAZARD VALUES

Once the data was compiled, a hazard value (HV) was calculated for each parameter following the protocols outlined by Swanson *et al.* (1997). HVs ranged between 0 to 5 for effect parameters and 1 to 2.5 for soil half-life and bioconcentration factor.

4.1 Human Health Hazard

Human health endpoints were assigned HVs on a scale of 0 to 5 according to severity. A value of 0 represented low toxicity while a value of 5 indicated high toxicity to human health. As discussed earlier, four endpoints were used to represent human health effects:

- rat oral LD_{50};
- rat inhalation LC_{50};
- carcinogenicity rating; and
- non-carcinogenic (NOAEL).

HVs for the oral LD_{50} (HV_{OR}) and inhalation LC_{50} (HV_{INH}) endpoints were calculated using a continuous, logarithmic-linear function. Cut-off values for the LD_{50} were established based on commonly accepted cut-off values (Davis *et al.* 1994, Swanson *et al.* 1997). The original cut-off values for the inhalation LC_{50} were set at >10,000 ppm and <31.6 ppm for assigning HVs of 0 and 5, respectively. However, since all the collected rat inhalation LC_{50}s were less than 1000 ppm, the cut-offs appeared to be inappropriate. Therefore, new cut-off values, consistent with the PMRA's protocol for pesticide labelling, were established. Accordingly, the rat inhalation LC_{50} cut-off values for setting HVs of 0 and 5 were > 2.0 mg/L and <0.05 mg/L, respectively. Table 2 illustrates the equations used to derive the HVs for the LD_{50} and LC_{50} endpoints.

Table 2: Equations used to derive hazard values from LD_{50} oral and LC_{50} inhalation data (Swanson *et al.* 1997)

Acute Oral Toxicity (HV_{OR})
If LD_{50} oral > 5000 mg/kg, $HV_{OR} = 0$
If LD_{50} oral ≤ 5 mg/kg, $HV_{OR} = 5$
For 5 mg/kg < LD_{50} oral ≤ 5000 mg/kg, $HV_{OR} = 6.165 - 1.666 \log(LD_{50}$ oral)

Acute Inhalation Toxicity (HV_{INH})
If LC_{50} inhalation > 2 mg/L, $HV_{INH} = 0$
If LC_{50} inhalation < 0.05 mg/L, $HV_{INH} = 5$
For 0.5 mg/L ≤ LC_{50} inhalation ≤ 2.0 mg/L
$HV_{INH} = 0.9395 - 3.121 \log(LC_{50}$ inhalation)

HVs for carcinogenicity (HV_{CAR}) were assigned based on the method shown in Table 3. As mentioned earlier, the carcinogenic ratings or information on which to base carcinogenicity ratings were obtained from IARC, RED, JMPR, IRIS, HSDB or the PMRA. If a carcinogenicity rating was not implicitly specified by a recognized authority or information was lacking to categorize an active ingredient based on expert judgment, the substance was assigned a default value of 1.5 for HV_{CAR} in accordance with recommendations made by Swanson and Socha (1997) regarding how to handle missing data in chemical ranking schemes. This default value (1.5) was chosen in place of the midpoint value (2.5) since 2.5 is not among the suite of carcinogenicity hazard values available (Table 3). Assigning a HV_{CAR} of 1.5 instead of 2.5 when carcinogenicity data is lacking offers a degree of conservatism without unrealistically inflating the contribution of carcinogenicity to hazard.

Table 3: Carcinogenicity scoring based on IARC and US EPA classifications (Swanson *et al.* 1997)

IARC classification	HV_{CAR}	US EPA classification	HV_{CAR}
Group 4	0	Group E	0
Group 3	0	Group D	0
Not Applicable (no IARC equivalent)		Group C	1.5
Group 2B	3.5	Group B2	3.5
Group 2A	4.0	Group B1	4.0
Group 1	5.0	Group A	5.0

HVs for non-carcinogenic effects (HV_{NCAR}) were determined using the oral NOAEL of a substance. In most cases, the NOAEL for the most sensitive species was selected to represent this endpoint. The NOAELs for some active ingredients (i.e. those in which a NOAEL was not established, a sub-chronic study was used to establish the NOAEL, the toxicological database was incomplete, or increased sensitivity to the young was apparent) were further reduced by dividing the NOAEL by an additional safety factor either recommended by a recognized authority or warranted by expert judgement. The equation shown in Table 4 was used to calculate HV_{NCAR}.

Table 4: Equations used to derive HV_{NCAR} values from NOAEL (Swanson 2000a)

Non - carcinogenic Toxicity (HV_{NCAR}) – Oral
If NOAEL oral > 1,000 mg/kg-day, $HV_{NCAR} = 0$ If NOAEL oral < 0.1 mg/kg-day, $HV_{NCAR} = 5$ For 0.1 mg/kg-day ≤ NOAEL oral ≤ 1,000 mg/kg-day, $HV_{NCAR} = 3.75 - 1.25 \log$ (NOAEL oral)

4.2 Environmental Hazard

Active ingredients were assigned HVs for their environmental effects. HVs for environmental effects also ranged from 0 to 5. A value of 0 represented low toxicity while a value of 5 represented high toxicity to the environment. Two endpoints were used to characterize a substance's environmental effects as follows:

- fish LC_{50} (acute aquatic); and
- water flea EC_{50} (acute aquatic).

HVs for acute aquatic toxicity to fish (HV_{AAF}) and water flea (HV_{AAD}) were calculated using 96-hour rainbow trout (*Oncorhynchus mykiss*) LC_{50} and 48-hour *Daphnia magna* LC_{50} or EC_{50} values, respectively, as illustrated in Table 5. The effect measurement for the EC_{50} was immobilization for *Daphnia magna*. A continuous, logarithmic-linear function was used to calculate both the HV_{AAF} and HV_{AAD} (Swanson *et al.* 1997). Commonly accepted cut-off values were chosen for the fish LC_{50}. The same cut-offs were applied to *Daphnia* EC_{50} values as supported by Snyder *et al.* (2000). With the exception of chloropicrin, LC_{50} and EC_{50} data were located in the specified species for all active ingredients considered. Since an EC_{50} for *Daphnia magna* was not available for chloropicrin, an EC_{50} for *Daphnia pulex* was used in its place.

Table 5: Equations used to derive hazard values from rainbow trout LC_{50} (Swanson *et al.* 1997) and *Daphnia magna* EC_{50} data (Snyder *et al.* 2000)

Acute Aquatic Fish Toxicity (HV_{AAF})
If $LC_{50} \geq 1000$ mg/L, $HV_{AAF} = 0$ If $LC_{50} < 1$ mg/L, $HV_{AAF} = 5$ For 1 mg/L ≤ $LC_{50} < 1000$ mg/L, $HV_{AAF} = -1.67 \log (LC_{50}) + 5.0$

Acute Aquatic Daphnia Toxicity (HV_{AAD})
If $EC_{50} \geq 1000$ mg/L, $HV_{AAD} = 0$ If $EC_{50} < 1$ mg/L, $HV_{AAD} = 5$ For 1 mg/L ≤ $EC_{50} < 1000$ mg/L, $HV_{AAD} = -1.67 \log (EC_{50}) + 5.0$

4.3 Exposure Potential

Three endpoints were used as surrogates for exposure potential as follows:

- soil half-life (persistence);
- aquatic bioconcentration factor (BCF); and
- release amount (exposure potential and route of entry).

Soil half-life and BCFs were assigned HVs ranging from 1 to 2.5. As with the effect parameters, higher HVs for exposure parameters represented a higher level of hazard and lower HVs represented a lower level of hazard in terms of environmental fate.

Table 6 illustrates the criteria used to determine HVs for soil half-life and aquatic bioconcentration. Calculations for the soil half-life HV (HV_{SOIL}) and aquatic bioconcentration HV (HV_{BCF}) were based on a continuous, logarithmic-linear scale to generate values between 1 and 2.5 (Swanson *et al.* 1997).

With the exception of thiophanate methyl, the soil or field dissipation half-life for each pesticide was used to reflect its soil half-life. Thiophanate methyl rapidly breaks down into the pesticide carbendazim in aerobic soil metabolism studies. The soil half-life for carbendazim (320 days) is much longer than that of thiophanate methyl (< 1 day). Consequently, to add a level of conservatism to thiophanate methyl's evaluation, the soil half-life for carbendazim was used. Considering the metabolite profile for only thiophanate methyl and not all other pesticides in the risk ranking was justified since this situation was unique to thiophanate methyl. For example, unlike other pesticide monographs, evaluations for thiophanate methyl were conducted in concert with its major metabolite, carbendazim. When comparing the physical/chemical and toxicological profiles for each of these pesticides, only the soil half-life was markedly different. Therefore, all other endpoints in the model were fulfilled using thiophanate methyl-based data.

Table 6: Equations used to derive hazard values from Soil half-life and Bioconcentration Factor (BCF) data (Swanson *et al.* 1997, Swanson 2000a)

Soil Half-life (HV_{SOIL})
If Soil $t_{1/2} \leq 4$, $HV_{SOIL} = 1$
If Soil $t_{1/2} > 500$, $HV_{SOIL} = 2.5$
For $4 <$ Soil $t_{1/2} \leq 500$,
$HV_{SOIL} = 0.311 \ln(\text{Soil } t_{1/2}) + 0.568$

Bioconcentration Factor (HV_{BCF})
If $\log(BCF) \leq 1.0$, $HV_{BCF} = 1$
If $\log(BCF) > 4.0$, $HV_{BCF} = 2.5$
For $1.0 < \log(BCF) \leq 4.0$,
$HV_{BCF} = 0.5 \log(BCF) + 0.5$

The release volumes were also factored into the exposure potential. As detailed in Section 5.2, the release volumes were used to generate a release-weighted risk score for each active ingredient. The simpler application of using HVs to yield a risk score is explained first, followed by a description of the more complicated process for yielding a release-weighted risk score.

5. 0 CHEMS MODEL APPLICATIONS

5.1 Risk Score

After HVs were calculated for each active ingredient, values were combined into an algorithm to obtain a risk score (RS) (Table 7). Following the risk paradigm of "Risk = Toxicity x Exposure", the sum of effect HVs were multiplied by the sum of exposure HVs to yield a RS as follows:

Table 7: Modified CHEMS Risk Score

Risk Score (RS) = (Human Health Hazard + Environmental Hazard) × Exposure Potential

Where: Human Health Hazard= $HV_{OR} + HV_{INH} + HV_{CAR} + HV_{NCAR}$

Environmental Hazard= $HV_{AAT} + HV_{AAD}$

Exposure Potential = $HV_{SOIL} + HV_{BCF}$

For any given pesticide, the total for human health and environmental effects could have a maximum score of 30. Exposure potential could receive a maximum score of 5, as each parameter could have a maximum value of 2.5. Theoretically, the maximum possible risk score for any given substance could be 150 (i.e. 30 x 5). A RS of 150 would indicate that a substance was extremely toxic, bioaccumulative and persistent in the environment. Conversely, a RS score of 5 would indicate that a substance generally had low toxicity, persistence and bioaccumulation potential.

5.2 Release-Weighted Risk Score

While the RS gives an indication of a substance's potential risk based on toxicity and physical/chemical parameters alone, the CHEMS model provides an opportunity to provide a more refined risk estimate by integrating release volumes into the model.

A simple approach for incorporating release volumes into the model would be to multiply the RS (Table 7) by the total release volume in kg (as approximated by pesticide sales data). However, the resultant risk ranking would likely be biased by the release amount. For example, risk scores theoretically range from 0 to 150 while release amounts for the pesticides examined ranged up to 436,000 kg. Consequently, a method for scaling the release amounts is needed to ensure that the releases do not dominate the algorithm.

To work around this, CHEMS devised a scheme to convert release data into release-weighting factors (RWFs) to reduce the contribution from release volumes in the algorithm. Further, to add another level of sophistication, instead of calculating one RWF representing total releases, the CHEMS model calculated media-specific RWFs. These RWFs were multiplied by effect HVs corresponding to the route of exposure to yield release-weighted hazard values (wHVs). The wHVs were then substituted for

effect HVs in Table 7, summed and multiplied by the sum of exposure HVs to yield a release-weighted risk score (WRS).

5.2.1 Determining Environmental Distribution

To proceed with the release-weighted risk ranking, a substance's environmental distribution must be known. To assist with this aspect, a Level III fugacity model was run for each active ingredient. Explanation of the Level III fugacity model is provided in Appendix 1. Based on 100% loading to soil, the Level III fugacity output provided the relative partitioning of each pesticide to air, water and land. The relative percentages to air, water and land derived from fugacity modelling were then applied to PEI's pesticide sales data to generate an environmental budget for each active ingredient.

5.2.2 Calculation of Release Weighting Factors

The amount of active ingredient deposited into each media, as determined by fugacity modelling, was converted into media-specific RWFs ranging from 1 to 10. RWFs were calculated for air (RWF_{air}), water (RWF_{water}), land ($RWF_{land+water}$) and total releases (RWF_{total}) as shown in Table 8:

Table 8: Calculation of release weighting factors

$$RWF_m = \ln [\text{release amount } (kg)_m] + a$$

where

$$a = 10 - \ln [\text{maximum release amount } (kg)_m], \text{ and}$$

$$m = \text{media of interest}$$

A method was developed to ensure that RWF values fell within a range from 1 to 10. By aking the natural logarithm of the release volume of each substance plus a constant (a), a ormal distribution of data points was produced. To ensure RWF values fell on a ormalized scale from 1 to 10 representative of their release volumes, a cut-off value was stablished based on calculations shown in Table 9. Any release volume below this cut-ff value would be assigned a RWF of 1. This procedure ensured that release volumes ess than the cut-off value would not produce a negative RWF or skew the resultant alues.

Figure 9: Calculation of Release Weighting Factor Cut-off Value

$RWF_m = 1$ for release amount (kg) $< b$

where

$b = e^{(1-a)}$

m = media

5.2.3 Calculation of Release-Weighted Hazard Values (wHV)

Once calculated, the media-specific RWFs were multiplied by their corresponding effect HVs to yield release-weighted hazard values (wHV) (Table 10). For example, HV_{INH} was multiplied by RWF_{air} since the general route of exposure by inhalation is through air. Similarly, the aquatic endpoints were multiplied by the RWF_{water} since aquatic organism exposure to chemicals occurs via water. The chronic endpoints (HV_{CAR} and HV_{NCAR}) were multiplied by RWF_{total} since over a lifetime an individual can potentially be exposed to the total amount of the chemical deposited in the environment, regardless of its partitioning. Finally, HV_{OR} was multiplied by $RWF_{land+water}$ since oral exposures can result through ingestion of water and soil.

The soil half-life and bioaccumulation parameters were not multiplied by RWFs as they already represent exposure potential.

Table 10: Release Weighting Factors Multiplied by Effect Hazard Values (Swanson *et al.* 1997)

$wHV_{OR} = HV_{OR} \times RWF_{LW}$	where:
$wHV_{INH} = HV_{INH} \times RWF_A$	wHV_X = release-weighted HV for term X
$wHV_{CAR} = HV_{CAR} \times RWF_T$	RWF_{LW} = land/water release weighting factor
$wHV_{NCAR} = HV_{NCAR} \times RWF_T$	RWF_A = air release weighting factor
$wHV_{AAF} = HV_{AAF} \times RWF_W$	RWF_T = total release weighting factor
$wHV_{AAD} = HV_{AAD} \times RWF_W$	RWF_W = water release weighting factor

5.2.4 Calculation of Release-Weighted Risk Score

After each endpoint was multiplied by its corresponding RWF, the wHVs then replaced the original HV_X values as shown in Table 11. This produced a release-weighted risk score (WRS) that integrated the release amounts for each pesticide.

Table 11: The Modified CHEMS Release-Weighted Risk Score

Weighted Risk Score = (Weighted Health Effects + Weighted Environmental Effects) × Exposure Potential

(WRS)

where: Human Health Effects = $wHV_{OR} + wHV_{INH} + wHV_{CAR} + wHV_{NCAR}$

Environmental Effects = $wHV_{AAF} + wHV_{AAD}$

Exposure Potential = $HV_{SOIL} + HV_{BCF}$

6.0 RESULTS AND DISCUSSION

The methodology outlined above was employed to yield relative risk rankings based on release-weighted risk scores and risk scores as shown in Table 12. For simplicity, only the ordinal ranks are shown. In addition, the ranks based on hazard, exposure and volume are provided for comparison.

To put the results into perspective, the first 2 rankings (i.e., release-weighted risk rank and risk rank) represent an estimate of risk since each of these rankings is based on a combination of hazard and exposure parameters. In the first column, release-weighted effects (sum of $wHV_{effects}$) were multiplied by exposure (sum of $HV_{exposure}$). The second column, risk rank, is based on the multiplication of effects (sum of $HV_{effects}$) by exposure. In contrast, the 3rd column (hazard rank) represents a relative ranking based on hazard (the sum of health and environmental hazard values) as no exposure parameters were used to determine these scores. The fourth column, exposure rank, is simply a ranking of the exposure scores derived from BCF and soil half-life. The last column, volume rank, provides a ranking of active ingredient sales in PEI for 2001.

According to release-weighted risk scores, the highest ranked substances include chlorothalonil, diquat dibromide, mancozeb, metiram, carbofuran, endosulfan, 1,3-dichloropropene, azinphos-methyl, paraquat and dimethoate.

The relative ranks for effects, exposure and volume can provide an insight into the drivers that influence the release-weighted risk rank. For example, it is not surprising that chlorothalonil ranked #1 for release-weighted risk given its relatively high ranks for effects, exposure and volume. Conversely, the low rank for carbathiin is anticipated given its low effects, exposure and volume ranks.

Table 12: Relative Rankings based on Release-Weighted Risk, Risk, Hazard, Exposure and Volume Scores

Active Ingredient	Release-Weighted Risk Rank	Risk Rank	Hazard Rank	Exposure Rank	Volume Rank
Chlorothalonil	1	4	4	11	2
Diquat dibromide	2	5	11	5	7
Mancozeb	3	22	12	28	1
Metiram	4	15	13	20	4
Carbofuran	5	3	1	15	19
Endosulfan	6	1	2	1	17
1,3 Dichloropropene	7	8	9	17	15
Azinphos-methyl	8	2	3	11	18
Paraquat	9	7	15	5	20
Dimethoate	10	21	10	28	10
Methamidophos	11	12	5	28	11
Thiophanate-methyl	12	17	25	8	12
Linuron	13	9	16	13	14
Metribuzin	14	23	21	14	8
Chloropicrin	15	11	6	27	27
Imidacloprid	16	14	19	7	13
MCPA	17	26	27	19	3
Thiabendazole	18	6	14	2	23
Metobromuron	19	24	23	16	9
Metalaxyl-M	20	28	28	18	6
Carbaryl	21	13	8	23	29
Thiram	22	18	17	21	31
Atrazine	23	19	20	10	26
Phosmet	24	16	7	26	24
Propiconazole	25	10	18	4	30
2,4-D	26	25	22	24	25
Fluazifop-p-butyl	27	20	26	3	21
Rimsulfuron	28	30	29	22	16
Hexazinone	29	29	31	9	22
Glyphosate	30	31	30	28	5
Carbathiin/carboxin	31	27	24	25	28

The third ranked substance, mancozeb, provides an example of the model's risk-discerning ability. In spite of its low ranks for effects and exposure, its high volume pushes mancozeb into the third spot for release-weighted risk. This outcome is expected considering, with the exception of chlorothalonil, mancozeb use is 1 to 2 orders of magnitude greater than all other actives ranked. This demonstrates the following risk principle: a substance with relatively low hazard and persistence can present a high risk to the environment if its environmental loading is high.

The ranking for carbofuran again demonstrates the model's risk-discerning ability. In spite of its low volume rank, its high ranking for effects and medium ranking for exposure collectively combine to raise its release-weighted risk rank to fifth highest. The

ranking for carbofuran illustrates another risk concept. A substance with low environmental loading but high hazard and medium persistence can pose a high risk to the environment.

The significance of incorporating release amounts into the algorithm is demonstrated when comparing the release-weighted risk rank to the risk rank. As shown in Table 12, the risk rank differs considerably from the release-weighted risk rank. For example, only 7 of the top 10 active ingredients identified in the release-weighted rank also appear in the top 10 of the risk rank. When release volumes are not integrated into the risk score, mancozeb, metiram and dimethoate all rank much lower. However, when environmental loadings are considered, all 3 of these actives move into the top 10. Similarly, linuron, thiabendazole, and propiconazole all rank in the top 10 when environmental loading is not considered. These observations convey the corollary of not including release amounts in the risk score.

While the exposure component of the risk score gives an indication of persistence once a substance is released into the environment, it does not replace environmental exposure. Unless new data is generated from testing or new QSARs are applied, the risk score, in effect, is a fixed score because it is based on measured or modelled toxicity and physical-chemical data. The release-weighted risk score, on the other hand, is subject to change following changes in pesticide use patterns. This approach is preferred since a substance's hazard and environmental presence are pivotal in risk determination. By including release amounts in the risk score, the release-weighted risk score provides a better proxy for exposure and, therefore, a better estimate of risk.

In spite of the clear cut ordering of risk suggested by the ordinal rank, the CHEMS risk ranking results should not be construed as a quantitative risk assessment. Rather, the CHEMS objective is to identify substances of high, medium and low risk. Following the model's precepts, categorizing the ranked actives into groups of high, medium and low risk is an acceptable practice to make the results more tangible. For example, expert judgement coupled with statistical cluster analysis could be used to identify relative groups using the weighted risk scores directly. If a hypothetical cluster analysis revealed statistically distinct groups for ranks 1-3, 4-9, 10-17 and 17-31, the pesticides in these groups could represent very high, high, medium and low risk pesticides, respectively.

Assuming that a statistical cluster analysis revealed the above pattern, based on 2001 pesticide sales, the highest-priority pesticides for future action (the ones that present the highest risk) would include chlorothalonil, diquat dibromide, mancozeb, metiram, carbofuran, endosulfan, 1,3-dichloropropene, azinphos methyl and paraquat. Before taking any regulatory action or introducing restrictive measures (i.e. banning, finding substitutes, or limiting the use of an active), more rigorous risk assessment methodologies above and beyond this preliminary risk ranking would need to be applied.

For example, a monitoring program for these actives could be implemented to discern which ones present the most risk to the environment. The exposure data collected from the monitoring study could be coupled with toxicity data to further characterize the risk

posed by each pesticide. In this way, the CHEMS relative risk ranking could help guide a prospective monitoring study, thereby assisting risk managers with managing more efficiently resources dedicated to mitigating risks posed by pesticides.

7.0 LIMITATIONS AND UNCERTAINTIES

Like all scoring and ranking systems, uncertainty is inherent in the CHEMS model. Most of the toxicity and fate data were measured (Table 13) and derived from reputable sources. In addition, when multiple values were available for an endpoint, the geometric or arithmetic mean was calculated to prevent outliers from biasing the estimate. The carcinogenicity ratings were for the most part obtained from recognised authorities; when ratings were not implicitly specified, there was sufficient evidence on which to base a carcinogenicity rating for most other actives. For the remaining 3 actives that lacked data to base their rating, these were assigned a default HV of 1.5 so as to not bias the results and underestimate the risk posed by substances lacking carcinogenicity data. Lastly, measured values were scarce for BCF. Consequently, the majority of data were estimated using a QSAR relating BCF to log K_{ow}. On the upside, the practice of employing K_{ow} values and K_{ow}-based QSARs to predict bioaccumulation potential is readily accepted by environmental fate experts when BCF data is unavailable (Environment Canada 2003).

Table 13: Number of measured, estimated and missing data points

Endpoint	# measured points (% of total)	# estimated[1] data points (% of total)	# missing data points (% of total)
Rat oral LD_{50}	31	0	0
Rat inhalation LC_{50}	31	0	0
Carcinogenicity	14 (45)	14 (45)	3 (10)
Non-carcinogenicity	31	0	0
Fish LC_{50}	31	0	0
Daphnia EC_{50}	31	0	0
Soil $t_{1/2}$	31	0	0
log Kow	31	0	0
BCF	12 (39)	19 (61)	0

[1] Estimated by QSAR or expert judgement.

While the CHEMS model is effective in its inclusion of environmental effects, health effects and fate parameters, it could benefit from the inclusion of additional hazard endpoints. For example, with the exception of the NOAEL and carcinogenicity rating, the analysis was largely based on acute measures. While immediate effects are of concern, the long-term effects of pesticides can have equally devastating results. As such, chronic endpoints should equally figure into the model. Modification to CHEMS could allow for the inclusion of some additional chronic endpoints (e.g. *daphnia* NOEC, avian NOEL, etc.) and this could help overcome this limitation.

With respect to environmental effects, the modified CHEMS model focuses on aquatic organisms. To make the environmental hazard assessment more complete, the CHEMS model could be expanded to include chronic and acute terrestrial endpoints (e.g. birds, mammals, plants, invertebrates, etc.). Finally, to round out the aquatic hazard assessment, the CHEMS model could be modified to include toxicity tests conducted on plants and amphibians.

On the release side, pesticide sales data was used as a proxy for pesticide use. While it would be preferred to have an accounting of every pesticide application made in PEI to accurately determine environmental releases, this data is not available. Therefore, based on application of pesticides carried over from previous year purchases or storage of current year purchases to the following year, it is possible that the sales data may have underestimated or overestimated the amount of pesticides applied in 2001. Regardless, based on a rolling pesticide inventory, the carry-over from previous years, or storage to succeeding years, on balance, the pesticide sales data, in the absence of actual applied amounts, is the best proxy for pesticide use.

Regarding environmental distribution, the fugacity multi-media model estimated environmental partitioning for each active ingredient based on its respective water solubility, vapour pressure, melting point and log K_{ow}. As with any model, the results are limited by the accuracy of the input data and the model's own set of limitations and assumptions. Most of the physical-chemical data used in the fugacity model were derived from the Pesticide Manual or Mackay Handbook. However, reliable estimates for some physical-chemical properties were not always available and the resultant fugacity output for these actives may have had more uncertainty associated with them. In addition, the fugacity model assumptions may not accurately reflect PEI's environment and/or the behaviour of the pesticides in this environment. For example, the fugacity model was run using the default values for media volumes, densities, organic carbon content for soil, bottom sediment and suspended sediment, advection rates for air, water, and soil, and reaction rates as modelled by Epiwin. Presumably, a more relevant environmental budget for each active may have been achieved if media-specific half-lives for each pesticide and environmental parameters that reflect PEI's environment were used in the fugacity simulations. However, considering that all the active ingredients were run using the same model assumptions, the uncertainty from these assumptions is somewhat negated since all actives were treated the same. Still, the biggest limitation for using the fugacity model lies in the fact that it is a model and, therefore, may not reflect a pesticide's actual environmental distribution. However, considering the costly and resource-intensive option of comprehensive measurement of all pesticide in soil, water and air, the fugacity model is a reasonable alternative for determining environmental distributions.

8.0 RECOMMENDATIONS

In spite of the limitations outlined above, the modified CHEMS risk ranking scheme provides a useful tool for prioritizing pesticides of concern for future action. The apparent clear-cut ordering of risk suggested by the relative risk rank should not be construed as a risk assessment. Rather, the results from CHEMS should be viewed as a quantitative risk ranking exercise used to guide future risk management activities with respect to pesticides.

Before taking any regulatory action, the pesticide in question should undergo a higher tier of risk assessment to confirm the preliminary results from the risk ranking exercise.

Some of the limitations of the CHEMS model include the heavy reliance on acute measures and the lack of acute and chronic terrestrial data. To round out the hazard characterization and strengthen the overall relative risk ranking in future iterations, the CHEMS model should be modified, where practically feasible, to include additional acute and chronic terrestrial and aquatic data.

In addition, to yield a more representative environmental budget for each active ingredient, future simulations of the fugacity model should be run using the media-specific reaction rates for each pesticide. This simulation would provide a superior characterization of the fate of pesticides in PEI's environment and thereby strengthen the overall relative risk ranking.

9.0 REFERENCES

Bintein, S., Devillers, J. and W. Karcher. 1993. Non-linear dependence of fish bioconcentration on n-octanol/water partition coefficient. *SAR QSAR Environ. Res.* 1:29-39.

Center for Clean Products and Clean Technologies (CCPCT). 1994. Comparative Evaluation of Chemical Ranking and Scoring Methodologies. Eds. Davis, G.A., Swanson, M. and S. Jones. Knoxville, Tennessee; University of Tennessee – CCPCT.

Environment Canada. 2000. A Risk Ranking of National Pollutant Release Inventory Substances in the Atlantic Provinces. Environmental Surveillance Report EPS-5-AR-00-3. July 2000.

Environment Canada. 2003. Guidance Manual for the Categorization of Organic and Inorganic Substances on Canada's Domestic Substances List. Determining persistence, bioaccumulation potential and inherent toxicity to non-human organisms. June 2003, Existing Substances Branch.

Hazardous Substances Data Bank. 2003. <http://toxnet.nlm.nih.gov/>

InfoPEI. 2004. <http://www.gov.pe.ca/infopei/Environment_and_Land/Water_Resources/Fish_Kill_Investigations_1994-2000/ >

International Agency for Research on Cancer. 2003. <http://www.iarc.fr/>

International Programme on Chemical Safety. Joint Meeting on Pesticide Residues (JMPR). 2003. <http://www.inchem.org/>

Mackay. D. 1991. Multimedia Environmental Models: The Fugacity Approach. Lewis Publishers, CRC Press, Boca Raton, Florida.

Mackay, D., Shiu, W. and K. Ma. 2000. Physical Chemical Properties and Environmental Fate Handbook. Chapman and Hall/CRCnetBASE.

Mutch, Jamie. 1999. Prince Edward Island Department of Technology and Environment. Relative Ranking of Acute Pesticide Risks to Fish. AGDEX 607/99-02.

Mutch, J., Ernst, W.R., Doe, K. G. and P. M . Jackman. 2000. Diagnosing the Cause of Frequent Fish Kills in Agricultural Areas of Prince Edward Island *in* Proceedings of 27th Annual Aquatic Toxicity Workshop: October 1-4, 2000, St. John's

Newfoundland, Canadian Technical Report of Fisheries and Aquatic Sciences 2331.

Ritter, L. 1997. Report of a Panel on the Relationship between Public Exposure to Pesticides and Cancer. *Cancer* 80: 2019-2033.

Snyder, E.M., Snyder, S.A., Giesy, J.P., Blonde, S.A., Hurlburt, G.K., Summer, C.L., Mitchell, R.R and D. M. Bush. 2000. 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. *Environ. Sci. Poll. Res.* 7(1):52-61.

Swanson, M.B., Davis, G.A., Kincaid, L.E., Schultz, T.W., Bartmess, J.E., Jones, S.L., George, E.L.. 1997. A Screening Method for Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts. *Environmental Toxicology and Chemistry* 16(2): 372-383.

Swanson, M.B., and Socha, A. (eds). 1997. Chemical Ranking and Scoring: Guidelines for Relative Assessments of Chemicals. Pensacola, FL; Society of Environmental Toxicology and Chemistry (SETAC).

Swanson, 2000a. Personal communication. Electronic mail to C. Roberts on December 4, 2000.

Tomlin, C.D.S. 2000. A World Compendium: The Pesticide Manual. (Ed.) CDS Tomlin. 12th Edition. The British Crop Protection Council, Binfield, UK, pp.1250.

USDA Pesticide Properties Database. 2003. <http://www.arsusda.gov/acsl/ppdb.html>

US EPA. 1995. Final Water Quality Guidance for Great Lakes System. Federal Register, Volume Number Thursday, March 23, 1995. pp. 15366-15425.

US EPA ECOTOX Database. 2003. <http://www.epa.gov/ecotox/ >

US EPA Exposure Tools and Software: EPI Suite v.3.10. 2003. <http://www.epa.gov/oppt/exposure/docs/episuitedl.htm >

US EPA Integrated Risk Information System. 2003. <http://www.epa.gov/iris/>

US EPA's Reregistration Eligibility Decision (RED) documents. 2003. <http://www.epa.gov/pesticides/reregistration/>

APPENDIX 1

Fugacity Multimedia Models

The Level I, II and III fugacity models are based on the work of Mackay (1991). While each model becomes generally more sophisticated with increasing levels, each model attempts to provide a picture of how a chemical partitions in the environment. In all cases, model simulation requires the input of chemical and environmental properties.

In the Level I simulation, the volumes and densities of all 7 media (air, water, soil, bottom sediment, suspended sediment, fish and aerosols), organic carbon content of soil, sediment and suspended sediment, fish lipid content and physicochemical properties (water solubility, vapour pressure, log K_{ow}, melting point) must be supplied. While these criteria are required for input, it is possible to run any fugacity model by using the assumptions for volumes, densities, organic and fish lipid content provided by the model developers. The Level I model describes how a fixed quantity of conserved (non-reacting) chemical introduced into the environment partitions at equilibrium between the 7 media listed above. In this iteration there is no consideration of reaction.

The Level II model adds another level of sophistication by requiring reaction rates for all media and advective flow residence times for air, water and sediment burial. As opposed to introducing a fixed amount of chemical, the Level II model simulates a situation in which a chemical is continuously discharged at a constant rate and a steady-state is achieved in which input and output rates are equal. The medium receiving the emission is unimportant, because the chemical is assumed to become instantaneously distributed at equilibrium condition. In addition to providing environmental distribution of the chemical, by including advection and reaction rates, the Level II fugacity provides an estimate of chemical persistence and identifies which loss processes will be most important in removing a chemical from the environment.

The Level III simulation requires data on intermedia transport velocities and takes into account the movement of chemical from one media to another in the calculation of environmental persistence. Unlike Level II, the Level III model does not assume equilibrium between media. This simulation provides a more realistic description of a chemical's fate including the important degradation and advection losses and the intermedia transport processes. The distribution of the chemical between media depends on how the chemical enters the system, (e.g. to air, water, or both) and the mode of entry affects the overall environmental persistence.

More information about fugacity modelling can be obtained from Mackay (1991).

APPENDIX 2 – RAW DATA AND REFERENCES

Information included in these tables is derived from 12 major references; these are cited throughout by the following abbreviations:

ECOTOX: United States Environmental Protection Agency. 2003. ECOTOX User Guide: ECOTOXicology Database System. Available: http://www.epa.gov/ecotox/. Retrieval May, 2003.

HSDB: Hazardous Substances Data Bank (database). 1998. National Library of Medicine. Bethesda, MD, USA. Available: http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB.htm. Retrieval May, 2003.

IARC: World Health Organization, 2003. International Agency for Research on Cancer (IARC). Summaries and Evaluations from 1972-2002. Available: http://www.iarc.fr/ . Retrieval May, 2003.

IH: Mackay, D., and W. Shui. 2000. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate of Organic Chemicals. Boca Raton, Florida. Lewis Publishers.

IRIS: U.S. Environmental Protection Agency. 2003. Integrated Risk Information System. Available: http://www.epa.gov/iris/. Retrieval May, 2003.

JECFA: Joint FAO/WHO Expert Committee on Food Additives. 2003. Monographs Series 38-50; Evaluations. Available: http://www.inchem.org/pages/jecfa.html. Retrieval May, 2003.

JMPR: Joint FAO/WHO Meeting on Pesticide Residues. 1965-2001. Annual Toxicological and Environmental Evaluations. Available: http://www.inchem.org/pages/jmpr.html. Retrieval May, 2003.

PC: A Chempendium of Information on Pesticides Used in Atlantic Canada. 1999. Environment Canada, Environment Protection Branch, Atlantic Region. 342 pp.

PM: Tomlin, C.D.S. 2000. The Pesticide Manual. 12th Edition. The British Crop Protection Council.1250 pp.

PMRA: Pest Management Regulatory Agency. 2003. Regulatory Notes. Available: http://www.hc-sc.gc.ca/pmra-arla/english/pubs/reg-e.html. Retrieval May, 2003.

PPD: USDA Pesticide Properties Database, 2003. Available: http://www.arsusda.gov/acsl/ppdb.html. Retrieval May, 2003.

Calculated: As estimated from log Kow based on the equation: log BCF = 0.91 * log Kow - 1.975 * log(6.8e-07 * Kow + 1.0) - 0.786 [Bintein 1993].

1,3 Dichloropropene	216	150-300	3	1) USEPA. 1998. Reregistration Eligibility Decision (RED): 1, 3 Dichloropropene. Prevention, Pesticides and Toxic Substances. EPA 738-R-98-016, December. 2) PM
2,4-D	558	400 - 764	6	1) JMPR 1996 2) PM 3) PC
Atrazine	2403	1869 - 3090	2	1) PM
Azinphos-methyl	11.6	4.4 - 25.4	19	1) USEPA. 1999. Human Health Risk Assessment: Azinphos-methyl. Health Effects Division (HED), Office of Pesticide Programs. May. 2) JMPR 1991
Carbaryl	400	225 - 850	7	1) USEPA. 2002. Updated Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED): Carbaryl. Prevention, Pesticides and Toxic Substances. PC Code 056801, May. 2) PM 3) PC
Carbathiin/Carboxin	3820		1	PM
Carbofuran	10	5 - 13.8	9	1) JMPR 1996 2) PM 3) PC
Chloropicrin	250		1	PM
Chlorothalonil	>5000		1	1) USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004, April. 2) PM
Dimethoate	364	180 - 600	6	1) USEPA. 1999. The Updated, Revised Health Effects Division (HED) Chapter of the Reregistration Eligibility Decision (RED): Dimethoate. Prevention, Pesticides and Toxic Substances. PC Code 035001, Case No. 0088, December. 2) PM 3) PC 4) JMPR 1996

Active	LD_{50} (mg/kg)	LD_{50} range	N	Reference
Diquat dibromide	360	214 - 810	5	1) JMPR 1993 2) PM 3) USEPA. 2001. Tolerance Reassessment Eligibility Decision (TRED) Document: Diquat Dibromide. Prevention, Pesticides and Toxic Substances. PC Code 032201, December.
Endosulfan	43.2	9.6 - 110	12	1) USEPA. 2002. Reregistration Eligibility Decision (RED): Endosulfan. Prevention, Pesticides and Toxic Substances. EPA 738-R-02-013, November. 2) JMPR 1998 3) PM
Fluazifop-p-butyl	3003	2451 - 3680	2	PM
Glyphosate	5600		1	PM
Hexazinone	1424	1200 - 1690	2	1) USEPA. 1994. Reregistration Eligibility Decision (RED): Hexazinone. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-022, September. 2) PM
Imidacloprid	494	380 - 650	7	1) JMPR 2001 2) PM
Linuron	2499	1500 - 4000	3	1) USEPA. 1995. Reregistration Eligibility Decision (RED): Linuron. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-003, March. 2) PM
Mancozeb	>5000		1	1) JMPR 1993 2) PM
MCPA	901	700 - 1160	2	PM
Metalaxyl-M	667		1	PM
Methamidophos	17	13 - 21	5	1) JMPR 1985 2) USEPA. 1998. EFED Risk Assessment for the Reregistration Eligibility Decision (RED) Document: Methamidiphos. Prevention, Pesticides and Toxic Substances. PC Code 101201, Case No. 0043, January. 3) PM
Metiram	8518	6500 - 10000	4	JMPR 1993
Metobromuron	2603		1	PM

Active	LD_{50} (mg/kg)	LD_{50} range	N	Reference
Metribuzin	1827	1100 - 2300	4	1) USEPA. 1998. Reregistration Eligibility Decision (RED): Metribuzin. Prevention, Pesticides and Toxic Substances. EPA 738-R-97-006, February. 2) PM 3) PC
Paraquat	171	100 - 344	9	1) USEPA. 1997. Reregistration Eligibility Decision (RED): Paraquat Dichloride. Prevention, Pesticides and Toxic Substances. EPA 738-F-96-018, August. 2) JMPR 1986 3) PM
Phosmet	151	93 - 310	7	1) JMPR 1994 2) PM
Propiconazole	1601	1211 - 2233	3	1) JMPR 1987 2) PM
Rimsulfuron	>5000		1	PM
Thiabendazole	3957	3100 - 5100	4	1) USEPA. 1999. The HED toxicology chapter for the Reregistration Eligibility Decision document (RED): Thiabendazole. Health Effects Division. PC Code 060101, October. 2) JECFA Series 49 3) PM
Thiophanate-methyl	6640		1	1) JMPR 1995 2) PM
Thiram	2654	1800 - 4000	5	1) JMPR 1992 2) PM

Rat 4-hour Inhalation LC_{50}

Active	LC_{50} (mg/L)	LC_{50} range	N	Reference
1,3 Dichloropropene	3.6	2.7 - 4.54	5	1) PM 2) USEPA. 1998. Reregistration Eligibility Decision (RED): 1, 3 Dichloropropene. Prevention, Pesticides and Toxic Substances. EPA 738-R-98-016, December. 3) International Programme on Chemical Safety (IPCS). 1,3 Dichloropropene. Environmental Health Criteria; 146. World Health Organization, 1993.

Active	LC_{50} (mg/L)	LC_{50} range	N	Reference
2,4-D	>1.8		1	1) PM 2) JMPR 1996
Atrazine	>5.8		1	1) PM 2) USEPA. 2001. Revised Toxicology Chapter of the Reregistration Eligibility Decision (RED): Atrazine. Prevention, Pesticides and Toxic Substances. January.
Azinphos-methyl	0.16	0.13 - 0.21	3	1) USEPA. 1999. Human Health Risk Assessment: Azinphos-methyl. Health Effects Division (HED), Office of Pesticide Programs. May. 2) JMPR 1991
Carbaryl	>3.4		1	USEPA. 2002. Updated Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED): Carbaryl. Prevention, Pesticides and Toxic Substances. PC Code 056801, May.
Carbathiin/Carboxin	>5		1	PM
Carbofuran	0.08		1	1) PM 2) JMPR 1996
Chloropicrin	0.040		1	1) HSDB
Chlorothalonil	0.09		1	USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004, April.
Dimethoate	>2		1	USEPA. 1999. The Updated, Revised HED Chapter of the Reregistration Eligibility Decision (RED): Dimethoate. Prevention, Pesticides and Toxic Substances. PC Code 035001, Case No. 0088, December.
Diquat dibromide	0.344	0.121 - 1.09	4	1) JMPR 1993 2) USEPA. 2001. Tolerance Reassessment Eligibility Decision (TRED) Document: Diquat Dibromide. Prevention, Pesticides and Toxic Substances. PC Code 032201, December.
Endosulfan	0.0768	0.0126 - 0.5	4	1) PM 2) USEPA. 2002. Reregistration Eligibility Decision (RED): Endosulfan. Prevention, Pesticides and Toxic Substances. EPA 738-R-02-013, November.

Active	LC_{50} (mg/L)	LC_{50} range	N	Reference
Fluazifop-p-butyl				
Glyphosate	>4.98		1	PM
Hexazinone	3.94		1	USEPA. 1994. Reregistration Eligibility Decision (RED): Hexazinone. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-022, September.
Imidacloprid	0.07		1	1) JMPR 2001 2) PM
Linuron	>6.15		1	1) PM
Mancozeb	>5.14		1	1) JMPR 1993 2) PM
MCPA	>6.36		1	PM
Metalaxyl-M	>2.29		1	PM
Methamidophos	0.0989	0.0632 - 0.2	3	1) PM 2) JMPR 1985
Metiram	>5.7		1	1) JMPR 1993 2) PM
Metobromuron	>1.1		1	PM
Metribuzin	>0.65		1	1) PM 2) USEPA. 1998. Reregistration Eligibility Decision (RED): Metribuzin. Prevention, Pesticides and Toxic Substances. EPA 738-R-97-006, February.
Paraquat	0.495	0.001 - 10	4	1) JMPR 1986 2) USEPA. 1997. Reregistration Eligibility Decision (RED): Paraquat Dichloride. Prevention, Pesticides and Toxic Substances. EPA 738-F-96-018, August.
Phosmet	>1.12		1	PM
Propiconazole	>5.8		1	PM
Rimsulfuron	>5.4		1	PM
Thiabendazole	>0.5		1	PM
Thiophanate-methyl	1.7		1	1) JMPR 1995 2) USEPA. 2001. Revised Toxicology Chapter for Reregistration Eligibility Decision (RED):Thiophanate-methyl. Prevention, Pesticides and Toxic Substances. Case No. 2680, March. 3) PM
Thiram	4.42		1	PM

Carcinogenicity Rating

Active	Carcinogenicity rating	References
1,3 Dichloropropene	B2	1) USEPA. 1998. Reregistration Eligibility Decision (RED): 1, 3 Dichloropropene. Prevention, Pesticides and Toxic Substances. EPA 738-R-98-016. December. 2) IARC 1999, Vol. 71. 3) IRIS 05/25/00
2,4-D	D	PMRA 2003. Personal Communication with Julia Popa, Information Officer, PMRA . Email dated Jan. 31, 2003.
Atrazine	3	1) IARC 1999, Vol. 73. 2) USEPA. 2001. Revised Toxicology Chapter of the Reregistration Eligibility Decision (RED): Atrazine. Prevention, Pesticides and Toxic Substances. January.
Azinphos-methyl	E	1) USEPA. 1999. Human Health Risk Assessment: Azinphos-methyl. Health Effects Division (HED), Office of Pesticide Programs. May. 2) JMPR 1991
Carbaryl	B2	1) USEPA. 2002. Updated Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED): Carbaryl. Prevention, Pesticides and Toxic Substances. PC Code: 056801, May. 2) JMPR 1996
Carbathiin/Carboxin	no information	default value (HV_{CAR} = 1.5)
Carbofuran	D	JMPR 1996
Chloropicrin	3	HSDB 2002
Chlorothalonil	B2	1) USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004. April. 2) IARC 1999, Vol. 73. 3) JMPR 1987, 1990
Dimethoate	C	1) USEPA. 1999. The Updated, Revised Health Effects Division (HED) Chapter of the Reregistration Eligibility Decision (RED): Dimethoate. Prevention, Pesticides and Toxic Substances. PC Code 035001, Case No. 0088, December. 2) JMPR 1996
Diquat dibromide	E	1) USEPA. 1995. Reregistration Eligibility Decision (RED): Diquat Dibromide. Prevention, Pesticides and Toxic Substances. EPA-R-95-016. July. 2) JMPR 1993
Endosulfan	D	JMPR 1998

39088-30-4, used as surrogate)		Assessment Review Committee, Health Effects Division (HED), Office of Pesticide Programs. P.C. Code: 110902, May.
Glyphosate	E	USEPA. 1993. Reregistration Eligibility Decision (RED): Glyphosate. Prevention, Pesticides and Toxic Substances. EPA 738-R-93-014, September.
Hexazinone	D	USEPA. 1994. Reregistration Eligibility Decision (RED): Hexazinone. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-022, September.
Imidacloprid	D	1) JMPR 2001 2) PMRA REG2001-11
Linuron	C	1) USEPA. 1995. Reregistration Eligibility Decision (RED): Linuron. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-003, March. 2) IRIS 10/01/1993
Mancozeb	B2	1) USEPA. 1999. Reregistration Eligibility Decision (RED): Triphenyltin hydroxide (TPTH). Prevention, Pesticides and Toxic Substances. EPA 738-R-99-010. September. 2) JMPR 1993
MCPA (2,4-D assessment used as surrogate)	D	PMRA 2003. Personal Communication with Julia Popa, Information Officer, PMRA. Email dated Jan. 31/2003.
Metalaxyl-M (Metalaxy, CAS RN: 57837-19-1, used as surrogate)	E	USEPA. 1994. Reregistration Eligibility Decision (RED): Metalaxyl. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-017. September.
Methamidophos	D	JMPR 1985
Metiram	B2	1) USEPA. 1996. Reregistration Eligibility Decision (RED): Nabam. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-035. January. 2) JMPR 1993
Metobromuron	no information	default value (HV_{CAR} = 1.5)
Metribuzin	D	1) USEPA. 1998. Reregistration Eligibility Decision (RED): Metribuzin. Prevention, Pesticides and Toxic Substances. EPA 738-R-97-006, February. 2) IRIS 12/01/1996
Paraquat	E	USEPA. 1997. Reregistration Eligibility Decision (RED): Paraquat Dichloride. Prevention, Pesticides and Toxic Substances. EPA 738-F-96-018, August.

Active	Carcinogenicity rating	References
Phosmet	C	1) USEPA. 1998. Toxicology Chapter for the Reregistration Eligibility Decision (RED): Phosmet. Prevention, Pesticides and Toxic Substances. PC Code 059201, January.
Propiconazole	C	1) JMPR 1987 2) PMRA REG2000-06.
Rimsulfuron	no information	default value (HV_{CAR} = 1.5)
Thiabendazole	C	1) USEPA. 2002. Reregistration Eligibility Decision (RED): Thiabendazole. Prevention, Pesticides and Toxic Substances. EPA738-R-02-xxx. October. 2) JECFA Series 39
Thiophanate-methyl	C	1) USEPA. 2001. Revised Toxicology Chapter for Reregistration Eligibility Decision (RED): Thiophanate-methyl. Prevention, Pesticides and Toxic Substances. Case No. 2680, March. 2) JMPR 1995
Thiram	3	1) IARC 1991, Vol. 53. 2) JMPR 1992

No Observed Adverse Effect Level (NOAEL)

Active	Supporting Study	NOAEL (mg/kgbw/d)	Additional Uncertainty Factor applied to NOAEL	Justification	Reference
1,3 Dichloropropene	2-year rat	2.5			USEPA. 1998. Reregistration Eligibility Decision (RED): 1, 3 Dichloropropene. Prevention, Pesticides and Toxic Substances. EPA 738-R-98-016, December.
2,4-D	1-year dog/2-year rat	1			JMPR 1996
Atrazine	6-month luteinizing hormone surge	1.8	10	increased sensitivity of young	USEPA. 2001. Revised Toxicology Chapter of the Reregistration Eligibility Decision. Atrazine (RED): Atrazine. Prevention, Pesticides and Toxic Substances. January.
Azinphos-methyl	1-year dog	0.15			USEPA. 1999. Human Health Risk Assessment: Azinphos-methyl. Health Effects Division (HED), Office of Pesticide Programs. May.
Carbaryl	1-year dog	3.1	3	LOAEL to NOAEL extrapolation (3X justified by RED)	USEPA. 2002. Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED): Carbaryl. Prevention, Pesticides and Toxic Substances. PC Code 056801, May.
					IRIS 07/01/1989

Active	Supporting Study	NOAEL (mg/kgbw/d)	Additional Uncertainty Factor applied to NOAEL	Justification	Reference
Carbofuran	4-week dog	0.22			JMPR 1996
Chloropicrin	90-day rat	8	3	subchronic to chronic extrapolation	HSDB 2002
Chlorothalonil	2-year rat	2			USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004, April.
Dimethoate	2-year rat	0.05			USEPA. 1999. Dimethoate: The Updated, Revised HED Chapter of the Reregistration Eligibility Decision (RED): Dimethoate. Prevention, Pesticides and Toxic Substances. PC Code 035001, Case No. 0088, December.
Diquat dibromide	2-year rat	0.19			1) JMPR 1993 2) IRIS 01/01/1995
Endosulfan	2-year rat	0.6	10	evidence for increased susceptibility of young, endocrine disruption, uncertainty regarding neuroendocrine effects in the young, need for a developmental neurotoxicity study	1) USEPA. 2002. Reregistration Eligibility Decision (RED): Endosulfan. Prevention, Pesticides and Toxic Substances. EPA 738-R-02-013, November. 2) IRIS 10/01/1994 3) JMPR 1998
Fluazifop-p-butyl	2-year rat	1			PM
Glyphosate	Developmental rabbit	175			USEPA. 1993. Reregistration Eligibility Decision (RED): Glyphosate. Prevention, Pesticides and Toxic Substances. EPA 738-R-93-014, September.
Hexazinone	1-year dog	5			USEPA. 1994. Reregistration Eligibility Decision (RED): Hexazinone. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-022, September.
Imidacloprid	2-year rat	5.7			JMPR 2001
Linuron	1-year dog	0.77			USEPA. 1995. Reregistration Eligibility Decision (RED): Linuron. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-003, March.
Mancozeb	2-year rat	3			JMPR 1993
MCPA	1-year dog	0.15	3	lack of a complete data base on chronic toxicity	IRIS 01/01/1991
Metalaxyl-M	2-year rat	2.5			PM
Methamidophos	1-year dog	0.05	10	no NOAEL established	IRIS 03/01/1991
Metiram	1-year dog	2.5			JMPR 1993
Metobromuron	2-year dog	3			PM
Metribuzin	2-year rat	1.3			USEPA. 1998. Reregistration Eligibility Decision (RED): Metribuzin. Prevention, Pesticides and Toxic Substances. EPA 738-R-97-006, February.

Active	Supporting Study	NOAEL (mg/kgbw/d)	Additional Uncertainty Factor applied to NOAEL	Justification	Reference
Paraquat	1-year dog	0.45			1) USEPA. 1997. Reregistration Eligibility Decision (RED): Paraquat Dichloride. Prevention, Pesticides and Toxic Substances. EPA 738-F-96-018, August. 2) IRIS 02/01/1991 3) JMPR 1986
Phosmet	2-year rat	1.1	3	Incomplete database. Lack of acute and subchronic neurotoxicity studies in rats.	USEPA. 1998. Toxicology Chapter for the Reregistration Eligibility Decision (RED):Phosmet. Prevention, Pesticides and Toxic Substances. PC Code 059201, January.
Propiconazole	1-year dog/2-year rat	3.6			1) JMPR 1987
Rimsulfuron	1-year dog	1.25			PM
Thiabendazole	1-year dog/2-year rat	10			1) USEPA. 2002. Reregistration Eligibility Decision (RED): Thiabendazole. Prevention, Pesticides and Toxic Substances. EPA738-R-02-xxx. October. 2) JECFA Series 39
Thiophanate-methyl	1-year dog	8			USEPA. 2001. Revised Anticipated Residues, Acute and Chronic Dietary Risk Assessments for Thiophanate-methyl (TM) and its Metabolites Methyl 2-benzimidazole carbamate (MBC) and 2-Amine-1-H-benzimidazole (2-AB). Office of Prevention, Pesticides and Toxic Substances. Chemical No. 102001, March.
Thiram	2-year rat/ 1-year dog	1			JMPR 1992

Rainbow Trout 96-hour LC_{50}

Active	LC_{50} (mg/L)	LC_{50} range	N	Reference
1,3 Dichloropropene	4.60	3.94 - 5.36	2	ECOTOX
2,4-D	5.5	1.4 - 47	5	ECOTOX
Atrazine	10.7	4.5 - 24	6	ECOTOX
Azinphos-methyl	0.0073	0.0029 - 0.028	15	1) ECOTOX 2) PM
Carbaryl	1.58	0.32 - 5.4	41	ECOTOX
Carbathiin/Carboxin	2.1	2 - 2.3	2	ECOTOX
Carbofuran	0.48	0.38 - 0.60	2	ECOTOX
Chloropicrin	0.02		1	ECOTOX
Chlorothalonil	0.0272	0.0076 - 0.103	13	1) ECOTOX 2) PM
Dimethoate	7.4	6.2 - 8.6	3	ECOTOX
Diquat dibromide	24.05	14.83 - 39	2	1) ECOTOX 2) PM
Endosulfan	0.00081	0.00017 - 0.0029	37	ECOTOX
Fluazifop-p-butyl	1.3		1	PM
Glyphosate	20.2	1.3 - 240	22	1) ECOTOX 2) PM
Hexazinone	453.3	146.7 - 1964	6	1) ECOTOX 2) PM
Imidacloprid	211		1	PM
Linuron	3		1	ECOTOX
Mancozeb	1.6	1.1 - 2.2	2	1) ECOTOX 2) PM
MCPA	145	91 - 232	2	1) ECOTOX 2) PM
Metalaxyl-M	121		1	1) ECOTOX
Methamidophos	25		1	ECOTOX
Metiram	0.502	0.229 - 1.1	2	1) ECOTOX 2) PM
Metobromuron	42.5	36 - 50.2	2	1) ECOTOX 2) PM
Metribuzin	83	42 - 147	4	ECOTOX

Active	LC_{50} (mg/L)	LC_{50} range	N	Reference
Paraquat	20	15 - 26	2	1) ECOTOX 2) PM
Phosmet	0.578	0.105 - 10	17	ECOTOX
Propiconazole	6.87	0.83 - 506	4	1) ECOTOX 2) PM
Rimsulfuron	390		1	ECOTOX
Thiabendazole	1.5	0.56 - 3.5	3	ECOTOX
Thiophanate-methyl	25.2		1	ECOTOX
Thiram	0.071	0.048 - 0.130	4	ECOTOX

Daphnia magna 48-hour LC/EC_{50}

Active	EC/LC_{50} (mg/L)	EC/LC_{50} range	N	Reference
1,3 Dichloropropene	0.75	0.09 - 6.2	2	1) ECOTOX 2) PM
2,4-D	152	25 - 389	3	1) HSDB 2) ECOTOX
Atrazine	33.9	6.9 - 115	3	1) ECOTOX 2) PM 10th edition
Azinphos-methyl	0.0018	0.0011 - 0.0044	5	1) ECOTOX 2) PM
Carbaryl	0.0151	0.0056 - 0.73	6	1) ECOTOX 2) PM
Carbathiin/Carboxin	84.4		1	1) ECOTOX 2) PM
Carbofuran	0.045	0.029 - 0.086	5	1) ECOTOX 2) PM
Chloropicrin	0.06		1	ECOTOX
Chlorothalonil	0.12	0.07 - 0.18	4	1) ECOTOX 2) PM
Dimethoate	1.075	0.560 - 2.90	8	ECOTOX
Diquat dibromide	0.0507	0.0022 - 1.17	2	1) ECOTOX 2) PM
Endosulfan	0.322	0.158 - 0.720	11	ECOTOX

Active	EC/LC50 (mg/L)	EC/LC50 range	N	Reference
Fluazifop-p-butyl (Fluazifop-butyl, CAS RN: 69806-50-4, used as surrogate)	*499.5*	*412.4 - 553.9*	3	1) ECOTOX
Glyphosate	66.0	2.95 - 780	4	1) ECOTOX 2) PM
Hexazinone	179	85 -442	3	1) ECOTOX 2) PM
Imidacloprid	85		1	1) PM
Linuron	0.45	0.12 - 1.91	6	1) ECOTOX 2) PM
Mancozeb	1		1	ECOTOX
MCPA	>180		1	ECOTOX
Metalaxyl-M	>113		1	ECOTOX
Methamidophos	0.071	0.026 - 0.27	3	1) ECOTOX 2) PM
Metiram	2.55		1	PM
Metobromuron	44		1	PM
Metribuzin	7.25	4.18 - 35	4	1) ECOTOX 2) PM
Paraquat	2.7	1.2 - 6.1	2	1) ECOTOX 2) PM
Phosmet	0.008	0.0056 - 0.0109	3	1) ECOTOX 2) PM
Propiconazole	5.6	3.2 - 11.3	3	1) ECOTOX 2) PM
Rimsulfuron	>360		1	1) ECOTOX 2) PM
Thiabendazole	0.6	0.31 - 0.85	3	1) ECOTOX 2) PM
Thiophanate-methyl	10.4	5.4 - 20.2	2	1) ECOTOX 2) PM
Thiram	0.21		1	PM

Soil Half-Life

Active	Soil Half-Life	Reference
1,3 Dichloropropene	54	USEPA. 1998. Reregistration Eligibility Decision (RED): 1, 3 Dichloropropene. Prevention, Pesticides and Toxic Substances. EPA 738-R-98-016, December.
2,4-D	7	PPD
Atrazine	120	USEPA. 2003. Interim Reregistration Eligibility Decision (IRED): Atrazine. Prevention, Pesticides and Toxic Substances. Case No. 0062, January.
Azinphos-methyl	32	USEPA. 1998. Preliminary Environmental Fate and Effects Risk Assessment for Azinphos-methyl. Prevention, Pesticides and Toxic Substances. Case No. 0234, January.
Carbaryl	5	USEPA. 2003. Interim Reregistration Eligibility Decision (IRED): Carbaryl. Prevention, Pesticides and Toxic Substances. Case No. 0080, June.
Carbathiin/Carboxin	1	PPD
Carbofuran	11	PPD
Chloropicrin	1	PPD
Chlorothalonil	18.75	USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004, April.
Dimethoate	2.4	USEPA. 1999. Environmental Fate and Effects Division (EFED) Revised Chapter for the Reregistration Eligibility Decision (RED): Dimethoate. Prevention, Pesticides and Toxic Substances. February.
Diquat dibromide	>1000	PPD
Endosulfan	99	USEPA. 2001. Environmental Fate and Effects Division (EFED) Risk Assessment for the Reregistration Eligibility Decision (RED): Endosulfan. Prevention, Pesticides and Toxic Substances. PC Code 079401, April.

Active	Half-Life	Reference
Fluazifop-p-butyl	20	PPD
Glyphosate	1.85	USEPA. 1993. Reregistration Eligibility Decision (RED): Glyphosate. Prevention, Pesticides and Toxic Substances. EPA 738-R-93-014, September.
Hexazinone	216	USEPA. 1994. Reregistration Eligibility Decision (RED): Hexazinone. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-022, September.
Imidacloprid	426	PMRA REG2001-11
Linuron	49	USEPA. 1995. Reregistration Eligibility Decision (RED): Linuron. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-003, March.
Mancozeb	2	PPD
MCPA	25	PPD
Metalaxyl-M (Metalaxyl, CAS RN: 57837-19-1, used as surrogate)	40	USEPA. 1994. Reregistration Eligibility Decision (RED): Metalaxyl. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-017. September.
Methamidophos	4	PPD
Metiram	20	PPD
Metobromuron	30	
Metribuzin	106	USEPA. 1998. Reregistration Eligibility Decision (RED): Metribuzin. Prevention, Pesticides and Toxic Substances. EPA 738-R-97-006, February.
Paraquat	1067	PPD
Phosmet	3	USEPA. 1998. Environmental Fate and Effects Division (EFED) for the Reregistration Eligibility Decision (RED): Phosmet. Prevention, Pesticides and Toxic Substances. PC Code 059201, April.
Propiconazole	53	PPD
Rimsulfuron	11	PPD

Active	Soil Half-Life	Reference
Thiabendazole	668	USEPA. 1999. Environmental Fate and Effects Division (EFED) Document for Reregistration Eligibility Decision (RED): Thiabendazole. Prevention, Pesticides and Toxic Substances. PC Code 060101, Case No. 2670, February.
Thiophanate-methyl	320	USEPA. 2001. Environmental Fate and Effects Division (EFED) Document for the Reregistration Eligibility Decision (RED):Thiophanate-methyl and its major degradate MBC (methyl 2-benzimadazolycarbamate). Prevention, Pesticides and Toxic Substances. May.
Thiram	15.2	PPD

Log K_{ow}

Active	Log K_{ow}	log K_{ow} range	N	Reference
1,3 Dichloropropene	1.82			PM
2,4-D	0.33			PM
Atrazine	2.58	2.05 - 2.80	21	IH
Azinphos-methyl	2.96			PM
Carbaryl	2.34	1.59 - 2.81	10	IH
Carbathiin/Carboxin	2.2			PM
Carbofuran	1.90	1.23 - 2.32	8	IH
Chloropicrin	2.09			IH
Chlorothalonil	2.92			PM
Dimethoate	0.64	-0.294 to 0.79	6	IH
Diquat dibromide	-4.6			PM
Endosulfan	4.74			PM
Fluazifop-p-butyl	4.5			PM
Glyphosate	-1.7			IH
Hexazinone	1.2			PM
Imidacloprid	0.57			PM
Linuron	3			PM
Mancozeb	1.33			US EPA Exposure Tools and Software: EPI Suite v.3.10. 2003. http://www.epa.gov/oppt/exposure/ docs/

				episuitedl.htm
MCPA	-0.71			
Metalaxyl-M	1.71			PM
Methamidophos	-0.8			PM
Metiram	0.3			PM
Metobromuron	2.41			PM
Metribuzin	1.6			PM
Paraquat	-4.5			PM
Phosmet	2.95			PM
Propiconazole	3.72			PM
Rimsulfuron	-1.47			PM
Thiabendazole	2.39			PM
Thiophanate-methyl	1.5			PM
Thiram	1.73			PM

Log BCF

Active	log BCF	log BCF range	N	Reference
1,3 Dichloropropene	0.87			Calculated
2,4-D	0.8	-5 - 1.3	6	IH
Atrazine	1.16	0.50 - 2	11	IH
Azinphos-methyl	1.91			Calculated
Carbaryl	1.26	0.0 - 1.53	4	IH
Carbathiin/Carboxin	1.22			Calculated
Carbofuran	2.07	2.07	2	IH
Chloropicrin	1.12			Calculated
Chlorothalonil	2.24	0.97 - 2.70	5	USEPA. 1999. Reregistration Eligibility Decision (RED): Chlorothalonil. Prevention, Pesticides and Toxic Substances. EPA 738-R-99-004, April.
Dimethoate	-0.3			Calculated

Active	log BCF	log BCF range	N	Reference
Diquat dibromide	-0.06	-0.15 - 0.01	2	USEPA. 1995. Reregistration Eligibility Decision (RED): Diquat Dibromide. Prevention, Pesticides and Toxic Substances. EPA-R-95-016. July.
Endosulfan	3.38	1.91 - 4.04	6	1) USEPA. 2002. Reregistration Eligibility Decision (RED): Endosulfan. Prevention, Pesticides and Toxic Substances. EPA 738-R-02-013, November. 2) IH
Fluazifop-p-butyl	3.29			Calculated
Glyphosate	-0.26	-0.42 to -0.28	2	USEPA. 1993. Reregistration Eligibility Decision (RED): Glyphosate. Prevention, Pesticides and Toxic Substances. EPA 738-R-93-014, September.
Hexazinone	0.31			Calculated
Imidacloprid	-0.27			Calculated
Linuron	1.61	1.53 - 1.69	3	USEPA. 1995. Reregistration Eligibility Decision (RED): Linuron. Prevention, Pesticides and Toxic Substances. EPA 738-R-95-003, March.
Mancozeb	0.42			Calculated
MCPA as amine salts	-1.43			Calculated
Metalaxyl-M (Metalxyl, CAS RN: 57837-19-1, used as surrogate)	-0.1	-0.22 to -0.008	2	USEPA. 1994. Reregistration Eligibility Decision (RED): Metalaxyl. Prevention, Pesticides and Toxic Substances. EPA 738-R-94-017. September.
Methamidophos	-1.05		1	USEPA. 1998. Revision of Environmental Fate and Effects (EFED) Risk Assessment for the Reregistration Eligibility Decision (RED) Document to Include Registrant's Comments: Methamidophos. Prevention, Pesticides and Toxic Substances. PC Code 101201, Case No. 0043, January.
Metiram	-0.51			Calculated
Metobromuron	1.41			Calculated
Metribuzin	0.67			Calculated
Paraquat	-4.88			Calculated

Active	log BCF	log BCF range	N	Reference
Phosmet	1.15	0.23 - 1.56	4	IH
Propiconazole	2.60			Calculated
Rimsulfuron	-2.12			Calculated
Thiabendazole	1.39			Calculated
Thiophanate-methyl	0.58			Calculated
Thiram	0.79			Calculated