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Agrochemical risk prediction and assessment: a review of models and tools

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Introduction

Managing the effects of agrochemicals in Victorian waterways requires far more information than we (as scientists and/or managers) can afford to directly measure for all the places and all the times, and all the agrochemicals of interest. Strategies and/or tools are therefore required to focus monitoring and risk assessment programs in a cost-effective manner, and to predict agrochemical concentrations and effects in locations that have never been directly assessed (or inadequately assessed).

To assess the risk of agrochemicals to aquatic ecosystems, information is required on the environmental fate of particular chemicals, their concentrations in the environment (exposures) and toxicity to aquatic organisms (as illustrated by the ecological risk assessment framework shown in Figure 1). The overall ecological risk can then be determined based on the general principle that risk is a function of toxicity and exposure (or likelihood of an adverse effect).

A large number of predictive tools and models are available to assist with all levels of the risk assessment framework, ranging from problem identification, exposure and toxicity analysis, and finally risk characterisation. The tools available range from simple risk scoring methods through to complex modelling, are designed for different purposes, and each has inherent strengths and weakness.

The various tools and models available could aid in the assessment of agrochemical risks to waterways in Victoria. However, prior to adoption the usefulness of these models/tools and the level of further development required for the specific Victorian environment needs to be assessed. This publication provides a summary of our review of available risk assessment models, including their advantages and limitations.

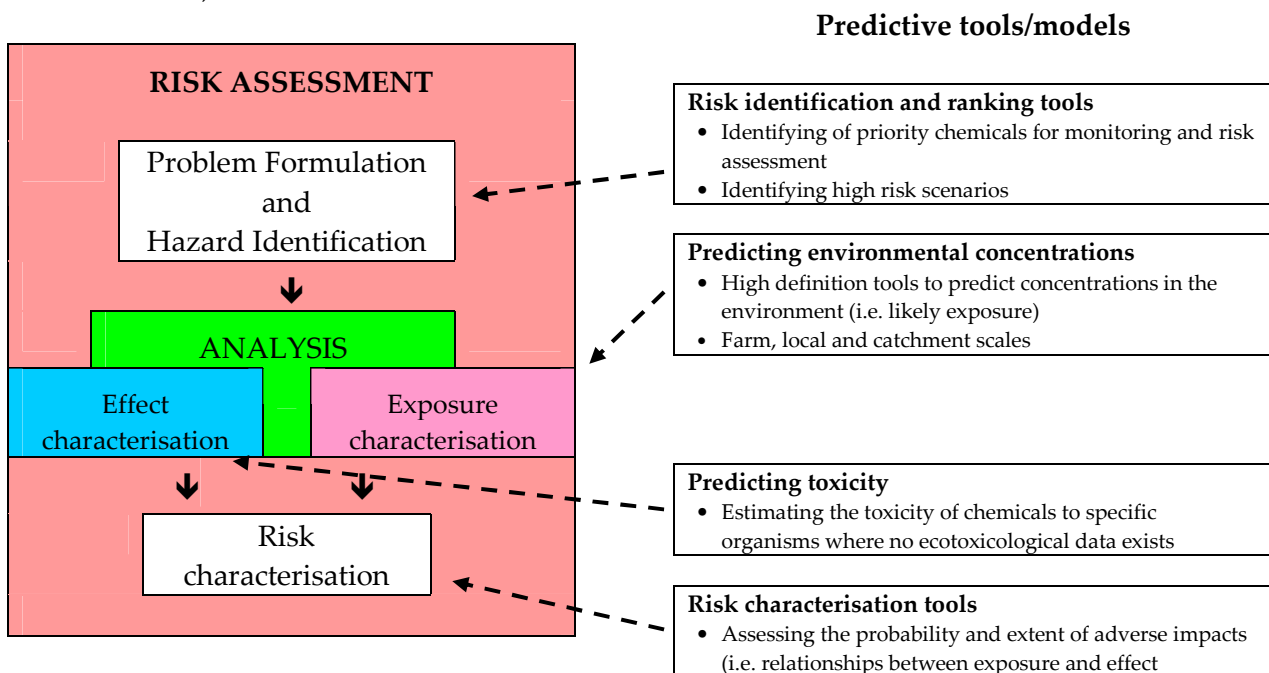


Figure 1 The ecological risk assessment framework and the main types of predictive tools/models available to assist with the various levels of risk assessment

Agrochemical risk scoring/ranking tools

To assist in identifying agrochemicals of concern within particular environments a range of risk scoring/ranking tools have been developed. These tools can assist in identifying high-risk agrochemicals to be targeted in monitoring programs or for further risk assessments. Risk scoring and ranking techniques rely primarily on the use of information on chemical properties, such as soil partitioning coefficient, solubility in water, and toxicity to aquatic organisms to generate a relative risk score or rank.

Pesticide Impact Rating Index (PIRI)¹

- Developed by CSIRO in Australia
- Primarily designed to rate the leaching risk posed by agrochemicals applied on a defined area of land
- Assists in selecting the agrochemicals to be targeting in monitoring programs, rather than predicting likely concentrations in the environment
- Can also be used for educating industry groups to understand potential impacts of chemical use selection
- A catchment-scale GIS version has also been developed.

Growsafe calculator

- Based on detailed modelling for key crops and soils in New Zealand
- Modelling has been interpreted into a user-friendly interface, requiring minimal input of information from the user, and predicts leaching and soil persistence risk.
- Tool is designed for use by growers to aid in chemical selection

University of Florida pesticide selection indices²

- These are guidelines provided to assist growers select pesticides that are less likely to impact on water quality.
- Indices are available for a range of crops.
- There are four key indices:
 - Relative leaching potential index (RLPI)
 - Relative runoff potential index (RRPI)
 - Toxicity index
 - Aquatic toxicity index

Pesticide Risk Management and Profiling Tool (ProMPT)³

- Evaluates pesticide fate in soil for any application rate and time of application for any land-based application anywhere in the world
- Is designed for use in situations where pesticides are spread over a large area, and is orientated towards the potential contamination of groundwater
- Uses a large set of public domain data to determine relative risks for pesticides.

Dutch Environmental Yardstick⁴

- Developed for assessing environmental impacts and is a points-based rating system
- The tool considers risks to water organisms, risk of groundwater contamination, and risk to soil organisms
- The tool is used as a decision tool by Dutch farmers for setting standards in ecolabelling and as a policy evaluation tool

ChemSCORER⁵

- Provides a rapid assessment of environmental hazards associated with organic chemicals
- Assesses chemicals for persistence, bioaccumulation potential, toxicity, and potential for long-range transport and ranks them against a set of reference chemicals

PestScreen⁶

- A ranking and scoring method developed as a screening tool to provide a relative assessment of pesticide hazards to human health and the environment
- Each hazard measure is scored, weighted and combined with pesticide application data to provide an overall indicator of relative concern (PestScore)

Environmental risk index⁷

- Developed to allow non-expert users to use leaching, persistence, toxicological, and bioconcentration data without needing knowledge related to each parameter for each agrochemical
- Linear models and quotient methods are used to calculate the environmental risk index.



Models predicting the fate of agrochemicals in the environment

In addition to the less complex risk scoring techniques, a range of higher definition models/tools are available for predicting the fate of agrochemicals in the environment. These higher definition models look to predict concentrations likely in specific environments and/or to quantify off-site losses. These tools focus on the three main pathways for off-site agrochemical movement, namely drift, leaching, and run off.

Spray drift models

AgDrift⁸

- Designed as a tool for evaluating the potential for buffer zones to protect sensitive aquatic and terrestrial habitats from undesired exposures resulting from aerial spray drift.
- Includes aerial spray drift, drift from ground rigs and from orchard/vineyard sprayers.
- Model has three tiers starting with basic predictions, based on assumed worst case situations to Tiers II and III, which allow for more variables to be manipulated.
- Ground spraying and orchard/vineyard spraying were later additions, and as such supporting data is limited.

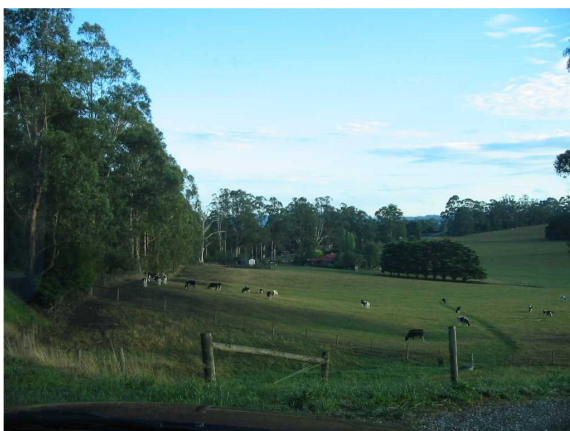
Models can be used to predict the extent of spray drift under various scenarios (ie application method and equipment)

German drift models⁹

- Predicts the concentration of chemicals drifting and assessing drift reducing equipment
- Modelling has been interpreting into 'drift values' based on a series of drift trials and available for field crops, fruit crops, grapevines and hops
- Enables assessment of drift reduction (ie through use of different sprayer)
- Specifically addresses risks to aquatic environments
- The German drift models show only the proportion of spray that settles out at each of various distances from a crop, not the total proportion of spray that drifts.

SprayCan¹⁰

- Predicts drift into neighbouring properties
- Based on AgDrift model
- Incorporates many site factors including spray equipment, wind direction and position of wind breaks.
- Rates the hazard associated with each prediction scenario
- Model predicts the risk to neighbouring enterprises, it does not specifically address contamination of water bodies
- Model only considers aerial spraying



Leaching of agrochemicals through or over soil into water

Leaching Estimation and Chemistry Models for Pesticides (LEACHP)¹¹

- Predicts the leaching of agrochemicals through soil profiles
- Ring testing has found LEACHP to predict leaching more accurately than other models.
- Model is complex and requires detailed data inputs and is only one-dimensional

PESTCRN3¹²

- Used to identify those chemicals likely to cause groundwater contamination and can be applied at an individual farm or at the catchment scale
- Addresses situations where groundwater recharge occurs at a variable rate

US EPA Models¹³

The US EPA has developed a suite of models to assess the movement of agrochemicals and to assist with chemical registrations and assessments:

- **PRZM-3** – predicts leaching through the crop root and unsaturated zone
- **3DFEMWATER** - models the flow and transport of contaminants through variably saturated media
- **PATRIOT** – used to assess the vulnerability of groundwater to pesticides
- **ADAPT** – simulates groundwater contamination, considers macropores
- **EXAMS** – evaluates the exposure of surface water to agrochemicals

GLEAMS¹⁴

- Used to assess the effect of farm management practices on the potential leaching of agrochemicals

Catchment scale models

Most of the models and tools developed to predict the fate of agrochemicals do so at a farm or very localised level. However there are also a number of models/tools for predicting agrochemical fate at the catchment scale.

National Water Quality Assessment Program (NAWQA) (USA)¹⁵

- The United States Geological Survey (USGS) have developed regression based models to establish quantitative linkages between pesticide concentrations measured at sampling sites and factors such as pesticide use, soil characteristics, hydrology and climate
- The models are known as Watershed Regressions for Pesticides (WARP) and are used to estimate the annual frequency distribution of pesticide concentrations at un-monitored streams

Canadian Fugacity Models¹⁶

- The fugacity models consider the partitioning of chemicals between soil, air, water, sediment and fish.
- The models determine the likely concentrations of chemical in each media based on the assumption that an equilibrium will be reached at some point in time
- Useful for assessing where chemicals are likely to end up (ie sediment or water column)
- The models enable the area to be defined, and so one can look at a small catchment scale or a large catchment scale.

Soil and Water Assessment Tool (SWAT)¹⁷

- SWAT is a catchment scale model developed to predict the impact of land management practices on water, sediment and agricultural chemical yields in complex catchments with varying soils and land use
- The model is physically based and requires input of specific information on weather, soil properties, topography, vegetation and land management
- SWAT enables users to predict long term (ie decades) impacts such as problems arising from the gradual build up of pollutants

Catchment Risk Assessment Tool (CAT)

- Developed to predict the off site impacts of local scale land use activities at both the farm and catchment scales
- CAT links site characteristics with catchment scale processes to yield outputs such as surface runoff, sediment loss, and groundwater discharge
- CAT was designed to assist in the understanding of spatial and temporal impacts of land use change.
- CAT in its current form can not predict the fate of agrochemicals

Catchment Modelling Tool Kit (CMT)

- The purpose of the tool kit is to enable prediction of the multiple impacts of land and water management decisions at a whole of catchment scale
- Tool kit includes the Catchment Management Support System (CMSS) used for strategic policy planning and the BC2C, SedNet, and E2 models for assessing water quality impacts at the catchment or sub-catchment scale.
- The tool kit does not specifically incorporate pesticides.

Risk characterisation tools

Whether the concentrations of agrochemicals within an environment have been measured directly or predicted through the use of models, risk characterisation is needed to assess these exposure concentrations along with available ecotoxicological effect data to determine the likelihood and nature of any adverse ecological impacts. Methods have been developed to assist with this risk characterisation step.

Risk Quotient Method

The Risk Quotient Method¹⁸ for risk assessment has been widely adopted by regulatory agencies internationally. The risk quotient method compares estimated environmental concentrations (EEC) relative to the toxicity of the agrochemical¹⁸. For example, if the EEC in a 15cm depth of water exceeds the concentration that would be toxic to a relevant species, then $Q > 1$ (where Q is an expression of estimated environmental concentrations). The quotient can be manipulated by altering the estimated environmental concentration, for example by reducing the frequency of applications. The APVMA considers that $Q < 0.1$ is low risk and no mitigation is required, $Q < 0.5$ to be an acceptable hazard, and that if Q is between 0.1 and 0.5, then some additional risk management might be imposed to further reduce Q. In addition to using predicted concentrations, the quotient method can also be used where measured concentrations are available.

Probabilistic risk assessment

In more recent times probabilistic risk assessment approaches have been adopted to aid in quantifying the likely risks posed. In probabilistic risk assessment, cumulative frequency distributions of both available ecotoxicological data and environmental concentrations are overlain. The overlap between the exposures and effects is then interpreted into a joint probability curve, which quantifies the likely risk. Some tools have been developed to assist with probabilistic risk assessment.

Probabilistic Risk Assessment Tools (PRAT)¹⁹

PRAT is a spreadsheet configured to receive exposure and effects data, convert this data, and to then generate an exceedence profile plot.

ETX²⁰

In terms of data input and output ETX is similar to PRAT however has been configured into a user friendly software program.

PERPEST²¹

Based on probabilistic principles, PERPEST predicts the effect of a pesticide on various community endpoints based on empirical data extracted from the literature. The user enters an environmental concentration for a particular chemical and other scenario based information, PERPEST then predicts the probability of effects on various grouped endpoints.

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