# Incorporating Environmental Fate Models into Risk Assessment for Pesticide Registration in South Africa

Report to the
**Water Research Commission**

by

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## EXECUTIVESUMMARY

The unintended effects of pesticides in the environment are of increasing concern to society. Implementation of a more rigorous risk assessment process during the registration of pesticides would significantly reduce the uncertainty related to the unintended effects of pesticides in the environment.

Pesticide registration in South Africa is regulated by the Fertilizers, Farm Feeds, Agricultural remedies and Stock Remedies Act (Act 36 of 1947) and is administered by the Department of Agriculture, Forestry and Fisheries (DAFF). According to the Act, an agricultural remedy or pesticide is defined as any chemical substance or biological remedy, or any mixture or combination of any substance or remedy intended or offered to be used for the destruction, control, repelling, attraction or prevention of any undesired microbe, alga, nematode, fungus, insect, plant, vertebrate, invertebrate, or any product thereof, but excluding any chemical substance, biological remedy or other remedy in so far as it is controlled under the Medicines and Related Substances Control Act (Act 101 of 1965), or the Hazardous Substances Act (Act 15 of 1973); or as plant growth regulator, defoliant, desiccant or legume inoculant, and anything else which the Minister has by notice in the Gazette declared an agricultural remedy (Act No 36 of 1947).

Risk assessment typically consists of an effect assessment that defines the concentration of a pesticide which is likely to pose a toxicity hazard to the environment and an exposure assessment which defines the predicted or expected concentration that is likely to occur in the environment, given specific conditions of use. These assessments are integrated to provide an indication of the likely risk associated with use of the pesticide. Given the large amount of data requirements for exposure modelling in particular, a tiered risk assessment approach is often adopted. The principle of this approach is, at the first tier, to initially perform a very simple risk assessment based on very conservative worst-case exposure input parameters and then, if necessary, refine this process using more realistic input parameters in subsequent steps (i.e. higher tiers). The need to move to a higher tier risk assessment is dependent on the risk outcome of the initial tier. If, under the conservative conditions of the first tier, no risk is expected, then there is no need to perform a risk assessment at the next highest tier using more data intensive inputs. The rationale behind this is that there is no point in performing a more detailed risk assessment if there is no risk using extreme worst-case exposure assessment data.

Lower tier assessments typically use very simple, conservative mass balance modelling approaches. Examples of these models are GENEEC2, EU Step 1, EU Step 2 and OECD Risk Indicator. Higher tier assessments utilise more realistic, complex models that consider the fate of the pesticide in the environment and the dynamics of the surface water ecosystem. PRZM is an example of a higher tier model. A tiered modelling system is designed to provide a thorough analysis of each pesticide, while at the same time focussing more detailed efforts on those pesticides that pose the greatest potential

risk. A Bayesian network was developed on the Netica platform, based on the OECD Risk Indicator model, while also explicitly accounting for uncertainty.

Field lysimeter studies were conducted to determine the fate and transport of pesticides maize and wheat cropping systems under South African soil and climatic conditions. For some pesticides, leaching concentrations were above the EU threshold of 0.1 µg/L. Even for those that were observed to leach at concentrations below the threshold, risk to the environment still exists, however. It is important to note that daughter metabolites were not measured, and these too can pose a risk to the environment. The fairly new Decagon G3 drainage gauges proved very useful to measure pesticide leaching, and further application of these devices in leaching studies is encouraged. The expensive SPES20 suction cups did not perform well under our trial conditions and are therefore not recommend for application in research under similar conditions. Further value can be added to these leaching data by using the drainage fluxes to estimate the loads of pesticide leached from fields. These data can also be extremely useful for the calibration and validation of pesticide leaching models.

Exposure scenarios were developed by considering the spatial variability of identified parameters in the South African landscape. The scenarios for exposure assessments should provide a reasonable representation of the conditions across the country, while also limiting the number of scenarios to a practical number. Since the impacts of agricultural chemicals on surface water resources are expressed in catchment areas, water management areas was a key consideration for the identification of scenarios. The First Edition of the National Water Resources Strategy (DWF, 2004) identified 19 areas (Figure 6-3), which provides a more representative coverage of climatic and physical conditions. The addition of one site (at Douglas) provides a more representative coverage of the Upper and Lower Orange Basins. For all 20 scenarios, default parameters were identified, such as soil characteristics for two soil profiles as well as rainfall.

A risk assessment framework is proposed, which consists of the following five components for each of the three Tiers:
1) The risk assessment is conducted for different environmental scenarios.
2) For each scenario, different application rates are considered.
3) The fate and transport of the applied chemicals are then assessed.
4) The resultant exported volumes are translated into concentrations in receiving waters.
5) The concentrations are compared to effects data to determine the risk

Finally, the Pesticide Water Calculator (PWC) model was parameterised for South African conditions. The model incorporates PRZM and Variable Volume Water Model and when the modelling results were compared to pesticide concentrations in field samples, the model provided very good estimations of exposure levels, which renders the model suitable for use at Tier I, whereas the model parameters can also be updated for more accurate predictions at Tier II and Tier III.

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## CONTENTS

## LIST OF TABLES

## LIST OF FIGURES

## ABBREVIATIONS

| | |
|---|---|
| ADI | Acceptable Daily Intake |
| AOAC | Association of Analytical Communities |
| APVMA | Australian Pesticides and Veterinary Medicines Authority |
| ARC | Agriculture Research Council |
| BN | Bayesian Net |
| CIPAC | Collaborative International Pesticide Analytical Council |
| CN | SCS Curve Number |
| DAFF | Department of Agriculture, Forestry and Fisheries |
| DEM | Digital Elevation Model |
| DoH | Department of Health |
| DSD | Droplet Size Distribution |
| DT50 | Half life |
| DWA | Department of Water Affairs |
| DWAF | Department of Water Affairs and Forestry |
| DWF | Department of Water and Forestry |
| e.g. | *exempli gratia* (latin) meaning “for example |
| EAS | Exposure Assessment Scenarios |
| EC50 | Concentration at which 50% of target organisms express the measured effect |
| EEC | Estimated Environmental Concentration |
| EFSA | European Food Safety Authority |
| EPA | Environmental Protection Agency |
| FAO | Food and Agriculture Organisation |
| FOCUS | FOrum for the Co-ordination of pesticide fate models and their USe |
| GC/MS | Gas Chromatography Mass Spectrometry |
| GLP | Good Laboratory Practice |
| GLC | Gas-Liquid Chromatography |
| HPLC | High Performance Liquid Chromatography |
| IPCS | International Programme on Chemical Safety |
| ISO | International Organisation for Standardization |
| Koc | Soil Organic Carbon-Water Partitioning Coefficient |
| LC50 | Concentration at which 50% of target organisms die |
| LOC | Levels of Concern |
| MCC | Medicine Control Council |
| MIC | Measured Insecticide Concentrations |
| MRL | Maximum Residue Limit |
| MS | Mass Spectrometry |
| NMR | Nuclear Magnetic Resonance |
| NOAEC | No Observed Adverse Effect Concentration |

| | |
|---|---|
| NOEL/C | No Observed Effect Level/Concentration |
| OC | Organic Carbon |
| OECD | Organisation for Economic Co-operation and Development |
| PEC | Predicted Environmental Concentration |
| ppb | Parts per billion |
| PRA | Probabilistic Risk Assessment |
| PWC | Pesticide Water Calculator |
| RACs | Regulatory Acceptable Concentrations |
| RQ | Risk Quotient |
| RSA | Republic of South Africa |
| SABS | South African Bureau of Standards |
| SCS | Soil Conservation Service |
| SDTF | Spray Drift Task Force |
| SWAT | Soil Water Assessment Tool |
| TER | Toxicity to Exposure Ratio |
| TLC | Thin Layer Chromatography |
| USA | United States of America |
| VVWM | Variable Volume Water Model |
| WHO | World Health Organisation |

# 1. INTRODUCTION

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## 1.1. Background

The unintended effects of pesticides in the environment are of increasing concern to society. This concern stems primarily from uncertainty related to the environmental effects of pesticides in the environment. Implementation of a more rigorous risk assessment process during the registration of pesticides would significantly reduce the uncertainty related to the unintended effects of pesticides in the environment.

In 2006 the Department of Agriculture and Forestry and Fisheries (DAFF, then the Department of Agriculture), published a pesticide management policy for South Africa (RSA, 2006) in which the Department acknowledged the need to minimise the risks posed by pesticides to human health and the environment. The policy specifically mentions the need to protect water quality through releasing fewer pesticides and/or less toxic pesticides into the environment and, secondly, to use practices that minimize the movement of pesticides to surface water and groundwater. One of the most important mechanisms to achieve this need is through the implementation of a rigorous risk assessment (based on sound scientific principles) during the pesticide registration process. This assessment should evaluate whether pesticide products submitted for approval for use in South African agriculture, pose an acceptable risk to the environment and human health, when used as directed.

Risk assessment typically consists of an effect assessment that defines the concentration of a pesticide which is likely to pose a toxicity hazard to the environment and an exposure assessment which defines the predicted or expected concentration that is likely to occur in the environment, given specific conditions of use. These assessments are integrated to provide an indication of the likely risk associated with use of the pesticide. Ideally, risk assessments should be based on a strong knowledge base – i.e. reliable and comprehensive data on the nature and extent of contamination, fate and transport processes, the magnitude and frequency of human and ecological exposure, and the inherent toxicity of all of the chemicals. However, in reality, information is often limited on one or more of these key data needed for risk assessment calculations. This means that risk assessors often have to make estimates and make use of modelling tools when performing risk calculations, and consequently all risk estimates are uncertain to some degree. For this reason safety factors are often built into the final risk assessment calculations to account for this uncertainty. Improved access to information that characterizes exposure and effects will therefore improve our ability to perform more reliable estimates of risk associated with various pollutants. These tools typically include monitoring and modelling data, fate and transport processes, spatial information on the use of hazardous pollutants and ecotoxicological methodologies that characterize toxicity.

Given the cost of conducting extensive field trials that monitor the fate and transport of pesticides under a variety of environmental conditions, international best practice currently advocates the use of fate and transport models to predict environmental concentrations for exposure assessment in pesticide registration. In the current risk assessment framework for registration of pesticides, DAFF does not utilize modelling tools to predict pesticide exposure in aquatic ecosystems under South African conditions. As such DAFF is unable to estimate or predict the likelihood and quantity of a pesticide that can move into non-target environments (e.g. ground- and surface water). Without adequately defining exposure, it is not possible to reliably assess the risk a pesticide poses to the environment. This research seeks to directly address this problem through the development of an improved risk assessment framework that integrates exposure and hazard to assess risk for the purpose of registering pesticides for agricultural use in South Africa.

The main focus of this research is to directly respond to the pesticide management policy by offering improved protection of the aquatic environment through improved risk assessment of agricultural pesticides. Outputs of this project will enable the regulator (DAFF) to make better informed decisions (based on sound scientific principles) related to pesticide registration that are intended to result in sustainable use of crop protection products that contribute to food security whilst posing minimal harm to the environment.

## 1.2. Methodology

Risk assessment consists of two fundamental processes. One is the hazard characterization, which relates to the toxicity of the chemical. This is typically achieved through toxicity tests that identify the chemical concentrations at which certain thresholds are exceeded (e.g. LC50, EC50). Generally the *Hazard Assessment* is achieved through rigorous toxicity testing procedures on standardized organisms. The second part of the risk assessment process is the *Exposure Assessment*, which aims to quantify the expected or predicted environmental concentration (PEC) of a chemical in the receiving environment under certain environmental conditions and conditions of use (e.g. application rates). The exposure assessment typically relies on fate and transport models, which integrate usage characteristics (e.g. the quantity or rate at which a pesticide is applied) with environmental fate properties of the pesticide (e.g. half-life, solubility, etc.) to provide an estimate of the PEC. An exposure assessment can be performed at varying levels of complexity ranging from simple worst-case predictions (e.g. “10% of the applied quantity of a pesticide moves into and adjacent water resource”) to more complex predictions that take the environmental fate of pesticides into account as well as environmental conditions that influence the movement of pesticides into water resources via runoff, leaching and spray drift. These may include soil properties, prevailing weather conditions (e.g. timing, frequency and intensity of rainfall events), and topography (e.g. slope.). The hazard and exposure assessment are combined to provide an indication of risk, whereby if the PEC exceeds the concentration deemed as hazardous, then an unacceptable risk is likely to exist. For the exposure

assessment a tiered system is often employed, whereby a simple worst case scenario is first adopted. If, under these conditions, no risk is expected, then there is no need to use more data intensive procedures. However, if at this first step, a risk cannot be ruled out, then a more detailed assessment takes place, using more realistic data inputs and environmental conditions to perform a more realistic risk assessment. The study was organised according to the following tasks:

**Task 1: Literature review**

This task evaluated the current risk assessment process used in the registration of pesticides in South Africa. In addition, risk assessment processes adopted in other countries were reviewed. In particular, the manner in which environmental exposure is predicted was reviewed (including the environmental fate and transport models and methods to standardize environmental data required as input into these models). The outcome of this review is a situation assessment and gap analysis of the current pesticide risk assessment process in South Africa in relation to current international best practice. The gap analysis highlights those steps or processes that are absent or inadequate to make a reliable assessment of the risk a pesticide poses to the aquatic environment under the current registration process and identify internationally accepted best practice approaches to address these gaps. This task identified specific models for use in exposure assessment which were considered for further evaluation in Task 2.

**Task 2: Model evaluation**

A number of models have been produced around the world and are routinely used in pesticide registration risk assessment. Task 1 identified models used to make estimates of pesticide exposure for the purposes of risk assessment. In order to determine the viability of using these models for risk assessment of pesticides in South Africa, it is essential that these models are interrogated so as to clearly identify their environmental and physicochemical data requirements and the availability of this data in South Africa. Where necessary the DAFF was consulted to determine the data supplied to them by chemical companies during the registration process and whether this meets the data requirements of the models. Through this process, data and knowledge gaps were identified and the feasibility of filling these gaps evaluated. In addition a sensitivity analysis of model data input, parameters were identified which have the most significant influence on model outputs. A sensitivity analysis involves varying input parameters independently (within realistic minimum and maximum ranges), one at a time, all other parameters being constant and observing the influence on model predictions. This identifies those model parameters for which reliable data needs to be sourced, for example physicochemical data (e.g. Koc and half-life) is often generated under international (e.g. European or North American) environmental conditions. If these parameters significantly influence the model outputs, then there is a justifiable reason to consider that this data be derived under South African conditions.

### Task 3: Development of exposure scenarios

A critical component of any modelling procedure is the identification of standardized relevant exposure assessment scenarios that represent typical or worst case environmental conditions under which pesticides may be applied. The primary purpose of defining standard scenarios is to increase the consistency with which industry and regulators predict pesticide exposure in surface waters. Furthermore, simulation models are often complex and are difficult to use properly. Having standard scenarios means that the user has less input to specify, and appropriate guidance simplifies the selection of these inputs. Worst case scenarios are desirable in that it represents a conservative estimate of pesticide exposure. Environmental conditions that influence the fate, transport and concentrations of pesticides in the environment vary widely across the spatial extent of a country. In order to integrate the use of environmental models into the regulatory decision making process, it was necessary to develop Exposure Assessment Scenarios (EAS) that are broadly representative of agriculture practiced in major production areas of the country. For example in the EU, ten different scenarios have been developed for use as data input into modelling, which are representative of typical environmental conditions in major agricultural production areas. These scenarios consider all relevant entry routes to a surface water body (e.g. runoff and spray drift) as well as all appropriate target groups, surface water situations, topography, climate, soil type and agricultural management practices. These scenarios are representative of a combination of worst-case situations in which off-target movement of pesticides would be expected to be highest. The objective of this task was to develop a standardized set of scenarios which are representative of different agrohydrological conditions in South Africa. These can then be used as input into environmental fate models to make estimates of Predicted Environmental Concentrations (PECs) for risk assessment purposes. Existing geographical resources, for instance Water Resources 2012 (Bailey and Pitman, 2016) and the Atlas of Climatology and Agrohydrology (Schulze et al., 2008), were considered in deriving scenarios for South Africa that represent different scenarios. Key environmental parameters that were considered for development of these scenarios include temperature, rainfall, crop type, soil texture and soil organic content.

### Task 4: Field Pesticide Dissipation Studies

Field studies were conducted to investigate whether environmental fate data generated in the European Union or USA could be used to make regulatory decisions in South Africa. Field trials were conducted in cropped as well as no-crop lands following the OECD Guidance document for conducting pesticide terrestrial field dissipation studies (OECD, 2016). The sites selected represent different soil types. At each site a minimum plot size of 2 x 5 $m^2$ should be used replicated at least four times. At each test site sampling should be done to 1 m depth and collected soil samples should be analysed for soil pH, soil type, organic matter, clay content and total percentage carbon. Pesticides used can include atrazine, mesotrione, methamidophos, methomyl, propiconazole, and cholorothalonil. The pesticides were applied at their recommended label rates. A tracer (e.g. Bromine)

can be applied with the tests compounds to determine the direction, depth and the rate of soil water movement in the treated soil.

Leaching and laboratory incubation trials were done at the University of Pretoria using the existing infrastructure. The drainage lysimeters situated at University of Pretoria experimental farm and that stationed outside of the university campus were used with low adsorption suction cups, wetting front detectors and soil water content sensors to monitor pesticides leaching concentrations. The data or results obtained from field dissipation studies can be compared with pesticides estimations generated by Pesticide Root Zone Models, e.g. PEARL, PELMO, PRZM and MACRO, etc. with the aim of determining how the models perform under South African conditions. The modelling estimation results can be compared with field test results and laboratory tests results and published data for the pesticides. The benefit of models is to help interpret the results of field dissipation study and the study's results can also be used to evaluate the model. The analytical equipment that can be used to analyse the pesticides used depending on the cost effectiveness of the instrument are GLC, HPLC and TLC and the instruments for identification purposes may involve MS, GC-MS, HPLC-MS and NMR.

**Task 5: Integration of Model Simulations into a Risk Assessment Framework**

The ultimate outcome of this task was to propose a risk assessment framework for registration of pesticides in South Africa that incorporates output from environmental fate models and toxicological data submitted as part of the registration process. Models recommended as part of Task2 and tested in Task 4 were used to estimate PECs for selected pesticides, using the exposure assessment scenarios developed in Task 3. The selection of pesticides for use in this assessment was done in collaboration with the DAFF. Outputs from the model simulations were incorporated into a risk assessment that compares toxicological data supplied by applicants during the pesticide registration process (e.g. LC50 values for an appropriate aquatic test organism such as *Daphnia magna*) to PECs through calculation of Toxicity to Exposure Ratios (TERs). TERs are typically compared to a trigger value (with safety factors built in to account for uncertainty), which if exceeded, represent an unacceptable risk to the aquatic environment. The magnitude of safety factors can be used to account for uncertainties in environmental fate modelling highlighted in Task 5 as well as those reported in the literature. Furthermore the extent to which variation in Koc and/or half-life influences the final risk assessment outcome (through repeated model simulations using realistic variations in these parameters) can also be considered when safety factors are derived to account for uncertainty.

The risk assessment process enables the regulator to make better informed decisions related to approval of use of pesticides in agriculture that take risks towards the aquatic environment into account. Relevant actions that may be taken based on the final calculated TERs could include: Approval of use (where TERs do not exceed trigger values for all exposure scenarios); or Spatially restricted use of a pesticide (where TERs exceed trigger values for some, but not all scenarios); or

The need for the applicant to perform more rigorous monitoring, modelling and ecotoxicological studies to demonstrate acceptable risk to the aquatic environment (where TERs exceed a trigger value for all exposure scenarios)

## 1.3. Expected Impact

The research is innovative in the South African context in that it aims to completely revise the manner in which pesticide risks are assessed during registration through use of best practice approaches in environmental risk assessment. Furthermore, the innovation of this research stands in contrast to previous WRC funded research on pesticides in water resources, where the majority of which have focused on understanding the occurrence and effects of pesticides already approved for use, many of which highlight the need for improved pesticide management. A major innovation in this research is that it shifts the concentration of research effort from reactive monitoring of pesticide effects associated with high uncertainty (i.e. pesticide risks are poorly understood due to a poor risk assessment during pesticide registration) to proactive regulation and management of pesticides through improved risk assessment processes at the point of registration. The use of environmental fate models in assessing the fate of pesticides in the South African environment is an innovation that has been explored in a limited number of research projects within South Africa, yet has not been taken to the next step through integrating their use in pesticide regulation. Successful implementation of this project's outcomes could lead to further innovation in assessing pesticide risks, by extending the methodologies and frameworks developed here to groundwater as well as to terrestrial environments. It should be noted that the proposed approach includes groundwater as a pathway for fate and transport, but the end point for exposure and effects assessment is surface water.

Through involvement of the DAFF, this project enhanced capacity development in a field in which DAFF had limited experience. A goal of the project is to develop DAFF staff to the point that they will make use of fate models and an improved risk assessment framework designed to afford increased protection to water resources from pesticides in South Africa.

# 2. LITERATURE REVIEW

*JM Dabrowski, M Thwala and T. Nepfumbada*

## 2.1. Background

The term “pesticides” is a collective term for a group of chemicals that include insecticides, herbicides and fungicides that are used to protect agricultural crops from insect and fungal pests as well as weeds. Every year thousands of tonnes of pesticides are applied to agricultural crops throughout the world. Pesticides are important to crop management because they contribute to increased crop yields and improve the quality of crops. While the benefits of pesticide use in improving crop quality and yields in agriculture are undeniable, these products are inherently toxic and are not species specific. Furthermore, pesticides tend to move from their point of application into non-target terrestrial and aquatic environments. The use of pesticides in agriculture therefore poses a threat to species in non-target environments and there are many such examples that have been published in the scientific literature (Schulz, 2004). The inherent toxicity of pesticides in combination with their intensive and extensive use requires careful regulation which should evaluate and mitigate the risk of agricultural pesticide use towards non-target organisms and human health prior to authorizing their use.

Regulation is typically enforced through the process of registering a pesticide for use, which the United Nations Food and Agricultural Organisation (FAO) defines as the process through which a responsible national government authority approves the sale and use of a pesticide following comprehensive scientific evaluation (FAO/WHO, 2010). The registration enables authorities to regulate the quality, use patterns, claims, labelling, packaging, and advertising of pesticides. The data required for the registration process are usually provided by the applicant (i.e. the manufacturer of the formulated pesticide). After application for registration the result may be a “provisional or full registration, with or without restrictions or conditions, or refusal of registration” (WHO, 2010a).

Information that is typically supplied by applicants during the registration process include: target pests, rate and frequency of application, efficacy data, toxicological data, ecotoxicological data and environmental fate data (i.e. physicochemical properties). This data is generally integrated into a framework that assesses the risk of the pesticide to human health and the environment when used under label instructions, with the ultimate goal being to ensure that only appropriate pesticides that pose acceptable levels of risk to human health and the environment enter the national market. The overall intent of the label is to provide clear directions for effective product performance while minimizing risks to human health and the environment and will generally include information on how to mix the pesticide, recommended dosage and application rates, the relative toxicity (e.g. very toxic, harmful, caution or unlikely acute hazard), restrictions on the method of application (e.g. aerial application using a crop-duster), safety precautions when handling and storing pesticides as well as information on risk to the environment.

Pesticides are typically evaluated according to a risk assessment framework and it can be argued that this process is even more important from the perspective of a developing country, as post-registration awareness building, training, compliance monitoring and enforcement tend to be relatively weak in many developing countries. The process of registration therefore offers the best opportunity to manage risks to the environment. Pesticide registration authorities in many developing countries generally have limited staff and relatively little experience in risk assessment approaches. This means that copying approaches for evaluating data provided for the purposes of pesticide registration as applied in countries with more resources is generally not an option.

In evaluating the risks of pesticides to the environment, both terrestrial and aquatic ecosystems and species representative of these ecosystems are typically considered. Within the aquatic ecosystem risks of pesticides to both ground and surface water resources are often accounted for. The scope of considering all of these environmental sinks is large and this review and project will focus on aquatic surface waters only. Furthermore, while the risk assessment framework presented here is applicable to numerous environmental stressors, the remainder of this review will focus on pesticides (including insecticides, herbicides and fungicides).

## 2.2. Pesticide Use in South Africa

South Africa is an agriculturally intensive country with a wide variety of crops produced across the country, ranging from grains (e.g. maize and wheat), deciduous, sub-tropical and citrus fruit; grapes, cotton, vegetables and sugar cane. The diversity of crops produced requires the use of a diverse array of pesticides, which has been one of the most important factors leading to increased yields and food security. From 1987 to 2009 there has been a slight increase in the total quantity of pesticides applied on an annual basis (21% increase over a 22 year period) (Table 2-1). From 2009 to 2014 however a significant increase in the total amount of pesticide applied was observed (25% increase over 5 years). This large increase was mainly attributable to large increases in the use of herbicides. The use of glyphosate alone increased by 6 tonnes from 2009 to 2014, presumably due to the increase in planting genetically modified, roundup-ready maize (Steenkamp, 2004).
The large quantities of pesticides used on an annual basis, in combination with their potential toxic effects and increasing trend of use, necessitates the need for improved regulation of pesticides in South Africa.

Table 2-1 Summary of pesticide use (kg x $10^3$) per category for the years 1987, 1991, 2009 and 2014.

| Pesticide | 1987[1] | 1991[2] | 2009[3] | 2014[4] |
|---|---|---|---|---|
| Herbicides | 8 640.68 | 8 083.48 | 9 273.447 | 19 218.70 |
| Fungicides | 4 423.75 | 5 526.66 | 7 751.48 | 4 683.66 |
| Insecticides | 4 225.23 | 5 291.78 | 4 755.98 | 5 229.78 |
| Total | 17 289.66 | 18 901.92 | 21 780.91 | 29 132.14 |

*[1]AIS (1987) [2]AIS (1991) [3]GfK Kynetec (2009) [4]GfK Kynetec (2014).*

## 2.3. Pesticide Regulation in South Africa

Pesticide registration in South Africa is regulated by the Fertilizers, Farm Feeds, Agricultural Remedies and Stock Remedies Act (Act 36 of 1947) and is administered by the Department of Agriculture, Forestry and Fisheries (DAFF). According to the Act, an agricultural remedy or pesticide is defined as any chemical substance or biological remedy, or any mixture or combination of any substance or remedy intended or offered to be used for the destruction, control, repelling, attraction or prevention of any undesired microbe, alga, nematode, fungus, insect, plant, vertebrate, invertebrate, or any product thereof, but excluding any chemical substance, biological remedy or other remedy in so far as it is controlled under the Medicines and Related Substances Control Act (Act 101 of 1965), or the Hazardous Substances Act (Act 15 of 1973); or as plant growth regulator, defoliant, desiccant or legume inoculant, and anything else which the Minister has by notice in the Gazette declared an agricultural remedy (Act No 36 of 1947).

The Act states that a fertilizer, farm feed, agricultural remedy or stock remedy shall be registered if:

- it is suitable and sufficiently effective for the purposes for which it is intended;
- and that it is not contrary to the public interest that it be registered;
- and the establishment where it is manufactured is suitable for such manufacture.

The manufactures or applicants are required to submit relevant or suitable data sets to the office of the Registrar of Act 36 of 1947 before any pesticide is placed on the South African market. As per the 2006 agricultural remedies regulations, the data sets listed below are required. Such data should be generated following relevant guidelines published by the by DAFF (2016a), the Department of Health (DoH), South African Bureau of Standard (SABS) or any other document or standards published in South Africa by any other department(s) or regulator(s) in the country.

The following studies are generally required for registration of new substances:

- Chemistry
- Toxicology (eco-toxicology and pharmacology)
- Environmental impact
- Residues
- Efficacy studies

Studies or reports on the determination of physical and chemical properties should be done according to Collaborative International Pesticide Analytical Council (CIPAC) or the Association of Analytical Communities (AOAC) methods. All safety studies such toxicology and residues should be done under the Organization for Economic Collaboration and Development Good Laboratory Practice (OECD GLP) accredited laboratories. Such studies should be done according to the latest guidelines for testing chemicals as published by the OECD and by the United States of America Environmental Protection Agency (US EPA) or any other recognized regulatory body such as the European

Chemicals Agency (ECHA), and the European Food Safety Authority (EFSA). Studies or reports on physical and chemical properties as well as formulation storage stability are compared with the most recent published guidelines (FAO/WHO, 2010b). Studies on physical and chemical properties should be done under International Organisation for Standardization (ISO17O25) or an OECD GLP accredited laboratory.

For all new active substance(s), the office of the Registrar of Act 36 of 1947 forwards the toxicological dossier to the DoH. The DoH conducts risk assessments of the substance under evaluation using human health and environmental safety criteria. The legislations followed by the DoH in this regard are Foodstuffs, Cosmetics and Disinfectants Act Number 54 of 1972 (FCD Act) and Hazardous Substances Act Number 15 of 1973 and their respective regulations. The Hazardous Substances Act mainly regulates the licensing of establishments that sell hazardous chemicals/substances and the classification of such chemicals following the WHO toxicity groups for specific formulations.

The DoH Directorate Food Control is responsible for conducting dietary risk assessment using human toxicological data sets submitted to the office of the Registrar of Act 36 of 1947. From the toxicological data, an Acceptable Daily Intake (ADI) is determined using the latest international standards. The DoH then estimates or calculates the Maximum Residue Limit (MRL) which is a statutory limit for the control of agricultural remedy/pesticide residues in food or raw agricultural commodities. The directorate Environmental Health Unit that resides in the DoH is responsible for conducting environmental health risk assessments. Both ecotoxicology and environmental fate data are forwarded to the DoH for the purposes of conducting both human and environmental health risk assessments using human health and environmental safety criteria.

Locally, generated field experimental efficacy and residue data sets are submitted to support the agricultural practice proposed on the product labels per crop commodity tested. Both efficacy and residues data sets are evaluated by the office of the Registrar of Act 36 of 1974. After evaluating the residues data, the DAFF proposes or determines the MRL supported by Good Agricultural Practice (GAP). The DoH publishes MRLs in a gazette issued under the regulations published according to the FCD Act.

The pesticide labels are approved after having been found to conform to the regulations relating to Agricultural Remedies (Government Gazette. No 29225 of 2006) and the requirements of the Guidelines of the Republic of South Africa (RSA), that is the Classification Code of Agricultural and Stock Remedies and Associated Labelling Practices.

All pesticides registered in South Africa are classified following the hazard classes published by the World Health Organization (WHO, 2010b). This is achieved by following guidelines for classification as developed by the International Programme on Chemical Safety (IPCS). In South Africa, agricultural remedies are categorized into five toxicity classes according to the formulation toxicity data for liquids

or calculations in case of solid formulations submitted with each formulation. The toxicity of the formulation is expressed as an LD50 value. The LD50 value is the lethal dose expressed in milligram per kilogram (mg/kg) body mass, which kill 50% of the test group of animals. The formulation toxicity class is assigned based of the following acute studies (oral rats LD50, dermal rats LD50, inhalation rats LC50, rabbits skin irritation, rabbits eye irritation and sensitisation in guinea pigs).

The DoH relies on expert opinion provided by Medicine Control Council (MCC) and other independent experts hired on a consultancy basis. After an expert opinion in the form of a risk assessment report provided to the DoH, the Director(s) of both Food Control and Environmental Health directorates forward letters either recommending or denying approval of any new substance or remedy. The Registrar of Act 36 of 1974, on behalf of the Minister of the DAFF, makes the final decision after taking into account other comments that may be received from other stakeholders in government and outside of government. In certain situations, the Registrar of Act 36 of 1974 grants conditional registrations due to lengthy delays encountered at the DoH. Conditional registrations are granted based on an independent toxicological risk assessment report prepared by a qualified toxicologist. All conditional registrations are renewable annually until such time a recommendation is received from the DoH.

The current risk assessment process used for registration of pesticides in South Africa is therefore largely focussed on human health effects and the establishment of MRLs for protection of consumers. While the DoH does consider environmental risks there are currently no guidelines prescribed for predicting environmental exposure and the potential risks that these could pose to aquatic and terrestrial organisms. To date the Registrar of Act 36 of 1974 has relied predominantly on expert opinion in considering potential risk to the terrestrial and aquatic environment.

**Data Submitted for Registration of an Active Ingredient for Use in Plant Protection**

This section provides details of the data required for the registration of pesticides as outlined in the application form for the registration of agricultural remedies as per agricultural remedies regulations published in the Government Gazette Number 29225 (2006).

Designation

- Common name
- Active ingredient(s) formulation
- Chemical name and group
- Chemical class
- Manufacturers development code
- CAS, CIPAC and other numbers
- Molecular structure, formula and mass

Physical and chemical properties of the active ingredient

- Physical state
- Colour
- Odour
- Density (at 20°C)
- Vapour pressure (at 20/25°C)
- Volatility
- Hydrolysis DT50 (days) for a measured temperature (°C) and pH.
- Solubility in water for a measured temperature (°C) and pH.
- Solubility organic solvents
- n-octanol/water portioning coefficient
- Boiling point (°C)
- Melting point (°C)
- Method of analysis and impurities

Toxicology studies of the active ingredient

- Acceptable Daily Intake (ADI)
- Acute oral LD50 (mg/kg rat/rabbit)
- Acute dermal LD50 (mg/kg rat)
- Inhalation LC50 (mg/L/hour rat)
- Skin irritation (rabbit)
- Eye irritation (rabbit)
- Sensitization (guinea pig)
- Reproduction (specify specifies)
- Sub-chronic toxicity (90 day NOEL mg/kg/day)
- Chronic toxicity (NOEL mg/kg/day)
- Carcinogenicity (life time) (NOEL mg/kg/day)
- Neurotoxicity NOEL (mg/kg/day)
- Teratogenicity NOEL (mg/kg/day)
- Mutagenicity/ Genotoxicity
- Metabolism (rat)

Ecotoxicology Data (Active ingredient – Technical grade)

Below is the list of ecotoxicological data (Table 2-2) required as outlined in the application form for the registration of agricultural remedies as per agricultural remedies regulations published in the Government Gazette Number 29225 (2006).

Table 2-2 Ecotoxicological data required for the registraion of a pesticide in South Africa

| Level | Test Organism | Toxicity Endpoint |
|---|---|---|
| Birds | Northen Bobwhite Quail and Mallard duck | Acute oral LD50 (mg/kg)<br>NOEL (mg/kg)<br>Reproduction |
| Fish | Bluegill Sunfish, Common Carb, Channel Catfish, Rainbow trout, etc. | LC50<br>NOEC<br>Reproduction toxicity<br>BCF |
| Aquatic Invertebrates | Daphnia | LC50 (mg/L)<br>NOEC (mg/L) |
| Aquatic Plants | Algae | LC50 (mg/L)<br>NOEC (mg/L) |
| Terrestrial Invertebrates | Earthworm<br>Soil micro-organisms | LC50 (mg/kg soil)<br>LC50 (mg/kg soil) |
| Pollinators | Bees | LD50 (µg/bees) |

Environmental Fate Data (Soil)

- Major metabolites
- Half life DT50 (days)
- Mobility
- Absorption
- Mobility of metabolites

Environmental Fate Data (Surface and Ground Water)

- Major metabolites
- Half life DT50 (days)

## 2.4. South African Pesticide Management Policy

In spite of the rigorous data required for pesticide registration, there are no established or published protocols or guidelines on how data supplied by applications to the registrar should be evaluated to determine risks to the environment in particular. While the procedure for developing ADI and MRLs for human health risk assessment is quite well established above, methods for evaluating environmental risks are not as advanced and, to date, the Registrar of Act 36 of 1974 has thus relied largely on expert opinion for evaluating environmental and ecotoxicological data submitted.

Although Act 36 of 1947 has been amended on several occasions, it has never been systematically revised. This was recognised in a Draft Pesticide Management Policy published by the Department of Agriculture (RSA, 2006), one of the main objectives of which was to minimise the hazards and risks of

pesticide use to human health and the environment. The policy highlighted a number of other important gaps that need to be addressed with regards to managing pesticide use in South Africa. These include (amongst others), the following:

- Of the more than 3 000 pesticides approved for use in South Africa, many have not been re-evaluated for years. Their safety therefore, has not been reassessed to bring them in line with today's more stringent standards of risk assessment.
- A change in the methodology in pesticide management is needed, based on a policy, which should take into account the necessary reduction of possible risks as well as sound production systems.
- The policy specifically mentions the need to protect water quality through releasing fewer pesticides and/or less toxic pesticides into the environment.
- The use of practices that minimize the movement of pesticides to surface water and groundwater.

One of the most important mechanisms required to address the gaps highlighted by the Pesticide Management Policy is the implementation of a rigorous risk assessment process which should integrate data supplied by applicants to evaluate whether pesticides products submitted for approval for use in South African agriculture, pose acceptable risk to the environment and human health, when used as directed.

## 2.5. Ecological Risk Assessment of Pesticides

Risk assessment is defined as a process that evaluates the likelihood that adverse effects may occur as a result of exposure to one or more stressors.

Ecological risk assessment is the process of characterizing and quantifying potential adverse effects on aquatic and terrestrial ecosystems following exposure to pesticides and chemicals and pollutants. It is a tool for regulatory decision-making for risk management (Rudén, 2006). The generally accepted global risk assessment framework typically consists of four steps (Figure 2-1). These include:

- Problem formulation (or hazard identification),
- Exposure assessment (which characterises the predicted or expected concentration that is likely to occur in the environment),
- Effect assessment (which characterises the concentration of a pollutant which is likely to pose a toxic hazard to target organisms representative of the environment) and
- Risk characterization (which integrates the exposure and effect assessment to provide an indication of the likely risk associated with use of the pesticide).

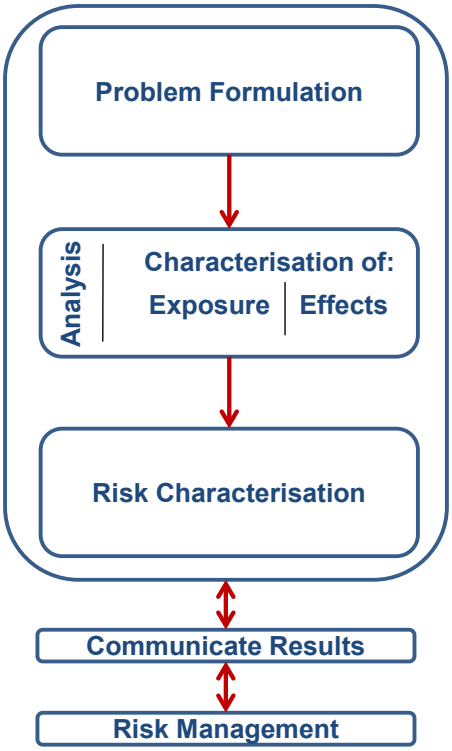


Figure 2-1 Ecological Risk Assessment framework (USEPA, 1998a).

Ideally risk assessments should be based on a strong knowledge base (i.e. reliable and complete data on the nature and extent of contamination, fate and transport processes, the magnitude and frequency of human and ecological exposure, and the inherent toxicity of all of the chemicals). However, in reality, information is often limited for one or more of these key data. This means that risk assessors often have to make estimates and make use of modelling tools when performing risk calculations, and consequently all risk estimates are uncertain to some degree. For this reason safety factors are often built into the final risk assessment calculations to account for this uncertainty. Improved access to information that characterizes exposure and effects will therefore improve our ability to perform more reliable estimates of risk associated with various pollutants. These tools typically include monitoring and modelling data, fate and transport processes, spatial information on the use of hazardous pollutants and ecotoxicological methodologies that characterize toxicity.

## 2.6. Problem Formulation

The problem formulation provides the foundation for the ecological risk assessment (USEPA, 1998a). It is an iterative process for generating hypotheses concerning why ecological effects are likely to occur as a result of human activities. The problem formulation defines the problem, describes the purpose and objectives of the risk assessment and provides a framework for regulatory action. The problem formulation should identify assessment endpoints that reflect management goals and the ecosystem they represent, develop a conceptual model(s) that represent predicted key relationships between stressor(s) and assessment endpoint(s) and provide a plan for analysing the risk.

### Assessment of Data Requirements

The problem formulation needs to identify important information and data that will be required to assess the risk of pesticides to the environment. These include the sources (i.e. identification of crops to which the pesticide will be applied), transport pathways, physicochemical properties and environmental factors influencing environmental fate and ecological effects of pesticides as well as the nature of the ecosystem(s) to be protected (e.g. terrestrial, ground- and surface water systems). This scoping process should also be used to identify missing data that may influence the reliability of the risk assessment.

Once the relevant input data have been identified, it is then important to assess the availability, quantity and quality of data inputs required for the risk assessment framework. Data of acceptable quality that is readily available leads to a risk assessment with comparatively low uncertainty and high confidence in its results. If data are limited, the associated uncertainties should be clearly accounted for in subsequent steps of the risk assessment process.

### Evaluate the nature of the problem

Risk assessments generally focus on the pesticide active ingredient. Assessments may also however consider pesticide formulations, inert ingredients and metabolites. This step of the problem formulation should describe the extent to which these related stressors will be included in the risk assessment, the rationale for their consideration, the methods used to evaluate the risks, and their contribution to the overall conclusions of the risk assessment (USEPA, 1998a).

The pesticide label application instructions (i.e. dosage and application rates) provide an indication of anticipated use and is an important input parameter for exposure models and for quantifying the magnitude of exposure to non-target organisms.

Information on ecological effects or toxicity of pesticides to non-target organisms is obtained from acceptable toxicity tests conducted on a limited number of organisms that serve as indicators for broad groups of animals and plants (e.g. the laboratory rat is the representative test species for mammals). Acute and chronic endpoints are selected from test data for the most sensitive species within these broad taxonomic groups. In addition to toxicity studies, alternate sources, including the scientific literature, can also be examined for toxicity data. Exposure data describe concentrations of pesticide that are expected to occur in the environment and are representative of the concentration to which aquatic organisms will be exposed. This data is typically obtained through field-based monitoring studies or via the use of environmental fate and transport models (i.e. simulated or predicted environmental concentrations).

### Select assessment endpoints

Assessment endpoints are used to estimate risk and should reflect the overall purpose of the risk assessment. In this respect, selection of assessment endpoints should consider two important aspects (USEPA, 1998a):

- Definition of suitable assessment endpoints which are understood as formal expressions of the environmental values to be protected
- Establishment of a certain level of protection which encompasses the acceptability of effects and the uncertainty linked to the prediction of effects.

The protection of species is a relevant assessment endpoint but difficult to evaluate and therefore not appropriate as a measurement endpoint. Due to the complexity of the matter, particularly when biodiversity issues are included, there are no agreed proposals on these points either in the scientific or in the regulatory community. In general, the sustainability of populations of non-target organisms should be ensured.

Typical assessment endpoints include reduced survival and growth, and reproductive impairments for individual animal species from direct acute and direct chronic exposures. For plants, the assessment endpoints are typically concerned with maintenance and growth of non-target species. Although these assessment endpoints are measured at the individual level, they indicate potential risk to populations.

### Prepare a conceptual model

The conceptual model consists of two components (USEPA, 1998a):

- a set of risk hypotheses that describe the predicted relationships between the pesticide, exposure, and assessment endpoint and
- a diagram that illustrates the relationships in the risk hypotheses.

Typical conceptual models are flow diagrams that contain boxes and arrows illustrating these relationships. Developing a conceptual model allows the risk assessor to identify the available information regarding the pesticide, justify the model, identify data and information gaps, and rank model components in terms of uncertainty.

### Develop an analysis plan

This is the final stage of problem formulation in which a plan for analysing data and characterising risk is developed (USEPA, 1998a). The analysis plan summarizes what has been done during problem formulation and targets those hypotheses that are likely to contribute to the risk. It also evaluates the risk hypotheses to determine how they will be assessed, develops the assessment design, identifies data gaps and uncertainties, determines which endpoints will be used to evaluate the risk hypotheses

(e.g. LC50, NOAEC, EEC's), and ensures that the planned analyses will meet the objectives of the risk assessment.

## 2.7. Exposure Assessment

For pesticide risk assessment, the exposure characterisation describes the potential for a plant or animal to come into contact with a pesticide. Ideally the exposure assessment should describe exposure pathways (i.e. routes of transport) and the magnitude, frequency and duration of exposure to pesticides (and metabolites) for each of these transport routes. The main output of an exposure assessment is the expected or predicted environmental concentration (PEC) of a pesticide in the receiving environment under certain environmental conditions and conditions of use (e.g. application rates).

The exposure assessment typically considers the most important transport routes for pesticides entering surface waters and integrates information on usage characteristics (e.g. the quantity or rate at which a pesticide is applied) and environmental fate properties of the pesticide (e.g. half-life, solubility, etc.) with other factors that influence transport (e.g. rainfall, soil properties, etc.) to provide an estimate of the PEC. Fate and transport models are often used in this assessment as field and catchment scale monitoring data that adequately characterise the multiple factors that influence pesticide transports is often limited (particularly for newly developed products). Given the large number of factors (and the inherent variability in these factors) that influence pesticide transport in the environment, there is generally a large amount of uncertainty associated with estimates of exposure.

**Pesticide Fate Data**

Exposure assessments typically require data on the fate of pesticides in soil, air, sunlight and water in order to predict how a pesticide will behave in the environment. This data is derived through laboratory and field experiments, the most important of which include:

- Persistence (expressed in terms of the half life – DT50)
- Water solubility
- Soil adsorption coefficient (Kd or Koc)
- Volatility
- Degradation products

Exposure assessments generally integrate environmental fate data and relevant environmental parameters that influence pesticide transport (e.g. slope, soil properties, rainfall data, etc.) in fate and transport models to characterise the behaviour or mobility of a pesticide and its potential to move into ground or surface water or bind to the soil. A final output of an exposure assessment is an estimated PEC. In deriving in-stream PECs, modelling will not only consider the fate and transport of pesticides once they are applied to a crop but also their fate once they have entered a modelled water resource

(i.e. partitioning of pesticides between water, sediment and plants). The flow rate and dimensions of the receiving water body and the total volume of water exposed to a pesticide input event is also important to consider in calculating a PEC. PECs are compared against relevant toxicity endpoints (see Effect Assessment section) in order to characterise the risk.

Environmental fate data should ideally be generated under conditions that would be expected to occur in the country/area where the pesticide is being registered. While this is often the case in countries from North America and the European Union this is not necessarily so for other countries. For example, while this data is required for registration of pesticides in South Africa, the data is often generated in countries outside of South Africa. There is often a degree of reservation about using physicochemical data from more temperate climates as combinations of the chemical properties as well as site-specific environmental conditions (e.g. soil properties, temperature, etc.) determine the fate and behaviour of pesticides (Daam and Van den Brink, 2010). These conditions vary greatly among different agro-ecological zones making the direct extrapolation of data between geographical regions very challenging (Ahmad and Kookana, 2007). However, Wauchope et al. (2002) found that while there is often variation in the Koc value of a specific pesticide (as an example), the values are adequate for discriminating between the relative mobility of a number of different pesticides. A study on the behaviour of three pesticides in South African soils reported similar Koc values to those reported in the international literature, while half-lives were generally longer in South African soils (Meinhardt, 2009). Other studies performed in South Africa have also shown good correspondence between Koc values and partitioning of pesticides between the sediment and water phase (Dabrowski et al., 2002b; Sereda and Meinhardt, 2005). These studies indicate that the European values provide a relatively good indication of pesticide behaviour in soils of South Africa and have been used successfully in predicting the relative mobility of pesticides under South African conditions (Dabrowski and Balderacchi, 2013).

**Pesticide Transport**

Estimating PECs for pesticides in water bodies is particularly challenging given that contamination occurs as a result of nonpoint source pollution. The main routes of transport are leaching, spray drift, drainage and runoff, each of which are influenced by a large number of highly variable environmental parameters (e.g. land use, land management, meteorology, soil properties, etc.), which, together with the physicochemical properties of the pesticide, must be taken into account in order to predict the transport of pesticides from agricultural fields into adjacent water bodies (Wauchope, 1978).

Spray drift and runoff are commonly regarded as the most important routes of entry for agricultural nonpoint source insecticide pollution into surface waters (Groenendijk et al., 1994) and may result in considerably different exposure scenarios (Erstfeld, 1999). Whereas spray drift leads to input of pesticides dissolved in the water phase, the contamination during runoff is sometimes largely as a result of pesticides associated with suspended particles (Mian and Mulla, 1992). Although pesticides

dissolved in the water phase pose more of an immediate toxicological threat, sediment associated pesticides have also been shown to adversely affect macroinvertebrate communities (Schulz and Liess, 2001). Leaching generally contributes to contamination of ground water and might affect surface waters only under specific geological conditions (Squillace et al., 1996).

**Runoff**

Surface runoff is the lateral movement of water from agricultural fields into adjacent water bodies and occurs when the precipitation rate exceeds the infiltration rate of the soil or when the length of a rainfall event exceeds the infiltration capacity of a soil. A complex interaction of a multiple number of variables ultimately influences the quantity of pesticide that can be expected to be present in surface runoff, the most important of which include; the time interval between the application of pesticides and the first heavy rainfall event; the slope and soil types of the catchment; the quantity of applied pesticide and the size and characteristics of vegetated buffer strips (Cole et al., 1997). Furthermore, runoff is highly dependent on the physicochemical properties of the pesticides themselves, which ultimately determine the amount of pesticide physically available to surface runoff (Blanchard and Lerch, 2000; Capel and Larson, 2001).

Pesticides can be found in two forms in surface runoff; in the soluble form (dissolved in runoff water) and in the eroded form (sorbed to suspended solids). The proportion and quantity of a chemical in each form at a given site depends upon the extent of sorption with the associated soil matrix, partitioning between runoff water and the suspended eroded material in transit and the degradation rate in the soil. Thus, important physicochemical properties to consider include the water solubility, half-life time and Koc. Pesticides with low water solubility tend to be more associated with suspended sediments as opposed to being dissolved in the water phase of the surface runoff.

Soil properties also play an important role in terms of the amount of surface runoff and the quantity of transported pesticide that occurs during an event. Soils with higher organic carbon content will tend to bind pesticides more than soils with low organic carbon content (Flury, 1996), while for any given precipitation amount, loamy and clay soils will give rise to a greater quantity of surface runoff (and hence pesticide loss) than a sandy soil, which will promote infiltration and leaching (Reus and Leendertse, 2000). Soils with high soil moisture content are more prone to runoff losses than sandy soils.

Slope has been shown to be the most important factor influencing runoff but can be greatly modified by the presence of vegetation (Wilcox & Wood, 1989). The timing of rainfall events in relation to the application date and half-life time of pesticides also plays a significant role in determining the amount of pesticide available in surface runoff. Studies have shown that the first heavy rainfall after application results in the highest quantity of pesticides in surface waters (Dabrowski et al., 2002a; Domagalski et al., 1997). Large rainfall events occurring a few days after the application of pesticides

have resulted in very high concentrations of pesticides being detected in the Lourens River (Schulz, 2001a).

### Spray Drift

Spray drift is the off-site movement of airborne pesticides at the time of application to any site other than that intended for application. Spray drift is one of the most important sources of nonpoint source pesticide pollution in edge-of-field surface waters, such as ditches, streams and ponds (Groenendijk et al., 1994; Holvoet, 2007). Due to the direct input of contamination, pesticide levels detected in adjacent water bodies are often high, posing a significant risk to aquatic fauna (Gilbert and Bell, 1988).

Pesticide drift can be difficult to manage because the full range of drift cannot be readily observed. Pesticides are most susceptible to spray drift when solutions are applied by ground spray equipment (i.e. tractors or portable handheld) but especially by aerial application. Many of the droplets produced by the nozzles during aerial application can be so small that they remain suspended in air and are carried by air currents until they contact a surface or drop to the ground. Applicator error can also cause drift but, even when pesticides are applied correctly, drift can still occur. As much as 30% of spray applications can move greater than 15 m from the intended site.

The tendency of a chemical to drift is influenced by a number of factors. These include the physicochemical properties of the individual pesticide, especially vapour pressure and boiling point as well as by droplet size and environmental parameters such as weather conditions (including wind speed and direction), topography, the crop area being sprayed and application characteristics. The proximity of water bodies from the pesticide application, the amount of pesticide drift, and toxicity of the pesticide are important factors in determining the potential impacts from drift. Pesticides with high vapour pressures are more difficult to keep on the application site and will almost always drift. Higher application rates also contribute to higher levels of drift. Maintenance of an effective buffer zone, which increases the distance between an agricultural field and an adjacent water body, is the most effective means of reducing contamination via spray drift.

### Leaching

Leaching is the movement of pesticides carried by water downward through permeable soils and affects groundwater (as opposed to surface water). In general most pesticides adsorb to soil particles (especially clay), become immobile, and do not leach. In contrast to surface water, groundwater does not continually dilute the contaminants that reach it. Flushing a plume of contamination from groundwater may take many years. The colder temperatures, limited microbiological activity, lack of sunlight and low oxygen levels that are found deep beneath the soil surface, slow chemical breakdown. The result is that there is very little, if any, breakdown of pesticides once they reach an aquifer.

Organic matter content is considered the single, most important soil property affecting pesticide breakdown by microorganisms (Flury, 1996). Organic matter in the soil provides more surface area for adsorption, increases the soil's ability to hold water and degrade pesticides, and nourishes microorganisms, all of which reduce pesticide leaching into groundwater. Soil organic matter can be increased by incorporating crop residues, adding manure, and growing cover crops.

The proportions of sand, silt, and clay affect the movement of water through soil (Stenemo et al., 2007; Meinhardt, 2009). Coarse-textured soils containing more sand particles have large pores and are highly permeable, allowing water to move through rapidly. Pesticides carried by water through coarse-textured soil are more likely to reach and contaminate groundwater. Clay-textured soils have low permeability. A soil containing large proportions of clay holds more water and adsorbs more chemicals from the water. This slows the downward movement of chemicals, helps increase the chance of degradation and adsorption to soil particles, and reduces the chance of groundwater contamination.

Loosely packed soil particles allow speedy movement of water through the soil. Tightly compacted soil holds water back like a dam, not allowing water to move freely through it. There are several ways that openings and channels can be created for water movement. For example, burrows dug by mammals and earthworms create openings for water to move. Plant roots penetrate soil, creating excellent water channels when they die and rot away. These openings and channels may permit relatively rapid water movement, even through some clay soils.

The amount of water already in the soil has a direct bearing on whether rain or irrigation results in the recharging of groundwater and possible leaching of pesticides into the aquifer. Soluble chemicals are more likely to reach groundwater when soil water content approaches or is at saturation.

Varying depths of soil separate the water table from the earth's surface. Soil protects the groundwater by providing an opportunity for pesticide adsorption and degradation, particularly in those layers at or near the soil surface. The greater the depth to the water table, the more protection the groundwater has from contamination. When the water table is high, or close to the surface, it is more vulnerable to contamination.

In addition to soil characteristics, the region's bedrock is another geological characteristic that has an important effect on the flow of recharge water and groundwater. Bedrock refers to the foundational layer beneath soil or rock fragments. The type of bedrock gives important clues to the fate of water. For example, limestone bedrock tends to have large channels from the surface to groundwater, allowing water to pass through quickly. Limestone close to the surface may allow quick passage of recharge water, reducing the chance for adsorption or degradation of chemicals to occur. Limestone also dissolves in water, creating underground passages and caves which let water move out of the area rapidly, possibly carrying chemicals long distances.

The topography of an area affects the speed with which water flows across the earth's surface. Steep slopes promote fast surface runoff and reduced chances for water to infiltrate into the ground. In valleys and flat areas, water flows more slowly across the surface, allowing more time for it to seep into the soil.

### Drainage

Agricultural drainage is the removal of excess water of the soil surface and/or soil profile of cropland, by either gravitational or artificial means. The two main reasons for improving the drainage of agricultural land are for (1) soil conservation through controlling salinization and (2) enhancing crop production through preventing water logging. In South Africa, drainage systems are most commonly associated with irrigated crops (Reinders et al., 2016).

Subsurface drainage systems consists of field drains, which can either be open ditches, or more commonly a network of drainpipes installed horizontally below the ground surface (Reinders et al., 2016). Subsurface drainage removes excess water from the soil profile, usually through a network of perforated tubes installed 0.6 m to 1.2 m below the soil surface. These tubes are commonly called "tiles" because they were originally made from short lengths of clay pipes known as tiles.

The most common type of "tile" is a perforated corrugated plastic tubing which allow water entry. When the water table in the soil is higher than the tile, water flows into the tubing, either through holes in the plastic tube or through the small cracks between adjacent clay tiles. This lowers the water table to the depth of the tile over the course of several days, allowing excess water to leave the field. In South Africa drain tiles are generally not flowing between June and October (Reinders et al., 2016).

In general the same environmental factors that influence leaching also influence drainage and pesticides can therefore end up being transported from the soil surface and crop root zone, through the soil profile into the drainage system. These drainage tiles typically discharge into a network of ditches excavated throughout the crop land and can eventually enter surface waters. In South Africa drainage could therefore be an important transport route in areas of intense irrigation.

### Exposure Assessment Models for Pesticides

Given the expense of conducting extensive field trials that monitor the fate and transport of pesticides under a variety of environmental conditions, international best practice currently advocates the use fate and transport models in order to predict environmental concentrations for exposure assessment in pesticide registration. As described above, pesticides can enter surface waters through runoff, spray drift, and drainage. Once pesticides have entered surface waters, they are exposed to a number of physical, chemical, and microbial processes that impact the fate of the pesticides. These processes include photodegradation, volatilization, biodegradation, absorption/adsorption, chemical degradation, leaching, and sedimentation. Models are used to predict the quantity of an applied

substance that moves from the point of application into and adjacent water body, taking these physical, chemical and microbial processes into account. The ultimate goal is to estimate a concentration of a pesticide that aquatic organisms may be exposed to (i.e. PEC).

These models range from simple screening models that require few inputs to more complex models that reflect the number of different factors that influence the fate and transport of a pesticide at a field scale. Data requirements typically required for running these models are those that influence the fate and transport of pesticides in the environment and are listed below.

Weather Data

- Daily Rainfall
- Daily Humidity
- Daily Temperature (minimum and maximum)
- Daily Temperature Variation
- Average Storm Duration

Soil Data

- Core Depth
- Bulk Density
- Soil Texture
- Field Capacity
- Wilting Point
- Organic Carbon

Field Management Data

- Field Slope
- Soil Erodibility
- Cropping Practice Factor
- Runoff Curve Numbers
- Cover Management Factors

Cropping Data

- Emergence Date
- Maturation Date
- Harvest Date
- Max. Interception Rate (Water)
- Max. Interception Rate (Pesticide)
- Rooting Depth

Physicochemical Data

- Soil/Pesticide Sorption coefficient
- Decay Rate
- Henry's Law coefficient
- Diffusion coefficient

### Exposure Assessment in South African Pesticide Registration

In the current risk assessment framework for registration of pesticides in South Africa, the DAFF does not utilize modelling tools to predict pesticide exposure in aquatic ecosystems and estimates of exposure are based entirely on expert opinion. As such the DAFF is unable to realistically estimate or predict the likelihood and quantity of a pesticide that moves into non-target aquatic environments. Given that toxicity data is provided in pesticide registration dossiers, deficiencies in the exposure assessment impose the most significant constraints in reliably assessing the risk a pesticide poses to the environment. A more detailed assessment of models and their data requirements and the availability of this data (i.e. through pesticide registration dossiers and other sources) is required to determine their suitability for use in South Africa.

### Exposure Assessment Scenarios

As highlighted above there are a number of weather, soil and other geographical factors that influence pesticide transport in the environment. These factors vary widely across the spatial extent of a country. Furthermore simulation models are often complex and are difficult to use properly. From a modelling perspective it is therefore impossible to account for and incorporate the high degree of natural variation in all of these input parameters when performing exposure assessments. To simplify this process a recognised approach is to identify relevant standardized exposure assessment scenarios that represent typical worst case environmental conditions under which pesticides may be applied. The primary purpose of defining standard scenarios is to increase the consistency with which industry and regulators predict pesticide exposure in surface waters. Having standard scenarios means that the user has less input to specify, and appropriate guidance simplifies the selection of these inputs. Worst case scenarios are desirable in that it represents a conservative estimate of pesticide exposure.

In the EU, ten different scenarios have been developed for use as data input into modelling, which are representative of typical environmental conditions in major agricultural production areas (FOCUS, 2001). These scenarios consider all relevant entry routes to a surface water body (e.g. runoff and spray drift) as well as all appropriate target groups, surface water situations, topography, climate, soil type and agricultural management practices. These scenarios are representative of a combination of worst-case situations in which off-target movement of pesticides would be expected to be highest. For example, agricultural areas experiencing high annual rainfall with steep slopes and soils with high clay

content demonstrate characteristics that would lead to relatively high inputs of pesticides associated with runoff. These areas can be considered to be representative of worst case runoff conditions and a favourable risk assessment derived using input data from these areas (for the exposure assessment) would therefore be protective of aquatic ecosystems in all agricultural areas (for runoff as a transport route). The use of worst-case scenarios therefore avoids the need to perform runoff simulations in areas where pesticide inputs associated with runoff would be expected to be relatively lower, which significantly reduces the burden on modelling effort.

## 2.8. Effect Assessment

Pesticides are by design meant to be toxic or to possess some bioactivity properties. Hence as part of pesticides risk management approach; environmental health regulators/risk assessors require that information pertaining to a pesticide's toxicological properties to humans and other organisms in the environment is provided by the applicant before the pesticide is registered. The regulators examine the provided information in order to ensure that under prescribed and intended conditions of use the pesticide will not pose unacceptable toxicity effects currently and in the future, and the examination is founded on the state of current knowledge. As new ecotoxicological information emerges; the conditions of use for an already registered pesticide might remain unchanged if the toxicity revels are still acceptable but might result to restrictions or even banning if the toxicity effects are found to be unacceptable.

Generally, the ecotoxicology effects information is assessed by analysing dose-response relationships from different endpoints across levels of organisation that indicate how toxic a pesticide or its active ingredient(s) is to different biota in the aquatic environments. The dose-response relationships are obtained from exposing biota (fungi, plants and animals) to varying exposure scenarios (concentration, acute, chronic), where the effect endpoints can include mortality/survival, reproduction and growth impairment, species diversity, etc. In order to harmonize the effects assessment process, standardized aquatic toxicity test protocols are adopted and the requirements may differ between countries.

### Data Requirements

The approach/pathway for the ecological effects assessment of pesticides and associated data requirements generally differs from country to country, however there are some standard toxicity effect endpoints that are commonly required for the aquatic ecosystem. The standard toxicity tests commonly adopted are those developed by the US EPA and OECD that focus on assessing effects to primary producers, primary consumers, and secondary consumers in aquatic ecosystems. For instance at the level of primary producers the EC50 and No Observed Adverse (NOAEC) effect levels are required for the *Pseudokirchneria subcapitata* and *Lemna gibba* as representatives for the algae and higher plants respectively. For invertebrates (primary consumers); the common requirements for the effects to pelagic invertebrates are the acute *Daphnia* 48 hrs LC50 (lethality) and EC50

(immobilization) as well as the acute *Penaeid sp*., tests. For the chronic effects the NOAEC on the reproduction, survival, hatching, growth and development rate endpoints of *Daphnia* and *Penaeid* are commonly required data.

Fish are used as model representatives for vertebrates (primary consumers). The 96 hours LC50s for rainbow trout (cold water species) and bluegill (warm water species) species are required data for the assessment of acute effects to invertebrates. The chronic effects are assessed based on the lifecycle effects reported as the NOECs for reproduction, hatching, growth and survival of eggs and hatchlings.

The briefly described data requirements are laboratory confined studies and often used in lower tiers of effects assessments. In some instances, where more refined and realistic data is required, more detailed field or microcosm studies may be required.

## 2.9. Risk Characterisation

Risk characterization is the final phase summary output of the ecological risk assessment and serves as the final input into risk management. The main purpose of the risk characterization process is to integrate the results of the exposure assessment and effect assessment to obtain an estimate of the level of effects that will result from exposure. In describing risk it is important to characterise the quality of data and uncertainties, assumptions, and strengths and limitations of the analyses;

For a risk characterization to be useful to risk managers, it must be transparent, clear, consistent, and reasonable. Once the risk characterization is finalized, it may be used as the basis for producing fact sheets, press releases, technical briefings, and other communication products.

The integration of exposure and assessment data can be based on a deterministic or probabilistic approach. The choice of approach needs to be decided upon during the problem formulation phase of the risk assessment, as this has a direct influence on data requirements for executing the exposure and effect assessment.

### Deterministic Risk Assessment

Deterministic methods are most commonly used to assess risk for the registration of pesticides. In this approach, a risk quotient (RQ) is calculated by dividing a point estimate of exposure (i.e. a single PEC value) by a point estimate of effects (i.e. relevant toxicity value). The calculation therefore integrates ecological effects (obtained during the exposure assessment) and exposure (pesticide use and fate and transport data) in quantifying risk. This ratio is a simple, screening-level estimate that identifies “risk” or “no risk” situations:

$$\frac{PEC}{Toxicity\ Value} < 1 \ \rightarrow No\ Risk$$

$$\frac{PEC}{Toxicity\ Value} > 1 \ \rightarrow Risk$$

The output is therefore a single point estimate of risk which could result in a simple “Yes” or “No” decision.

A major disadvantage of this method is that a single exposure and effect endpoint is used to make a decision on the potential risk that could be expected to occur in a natural field situation. This incorporates a large amount of uncertainty into the risk assessment calculation as there is inherently a large amount of variability in factors that influence both of these endpoints that may therefore not be adequately considered in evaluating true risk. Single point estimates of exposure (i.e. PEC value) derived from environmental fate and transport models used in exposure assessment are particularly uncertain due to a number of reasons (Dubus et al., 2003b):

- Spatial and temporal variability of environmental variables (e.g. physicochemical properties, soil properties and climatic and geographical factors) that influence model results.
- Uncertainty originating from difference in field sampling methods used to determine physical or chemical properties of pesticides
- Uncertainty in spatially referenced data
- The choice of model used to predict environmental concentrations, with some studies indicating that the variability in model results due to model selection could be more significant than that due to input parameter variation.

From an effect perspective different species exhibit differing sensitivity to chemical stressors. There is also intra-species variation depending on the life-stage of the test organism. It is for this reason that deterministic methods generally apply “worst-case” exposure scenarios and use sensitive species in deriving toxicity data in attempt to ensure the risk assessment is protective of all species. In addition, toxicity values are often divided by an assessment factor (e.g. 10 or 100 for chronic and acute values, respectively) to account for uncertainties in extrapolating effects observed in the laboratory to those that can be expected to occur in the field.

In summary, deterministic methods are relatively simple to execute and interpret and can be used to determine what is safe and is most likely protective of the environment. There is however a large amount of uncertainty associated with the method, it is not predictive and could also be too conservative (or over-protective) which could lead to certain beneficial products not being approved for use in agriculture.

**Probabilistic Risk Assessment**

Although the deterministic or risk quotient method is useful for screening purposes, it provides only one point estimate of environmental risk. A more detailed approach is to use probabilistic tools and methods to estimate the variability and/or uncertainty in factors that influence risk and to express risk in terms of the probability and magnitude of adverse effects. A probabilistic risk assessment (PRA) produces a distribution or range of exposure and effect values instead of one fixed value. In the example provided (Figure 1 2), the concentration at which 10% of species toxicity values will be exceeded is approximately 60 µg/L (Fig. 2-2). Approximately 95% of all exposures (water concentrations in the example) would be expected to be equal to or less than this value. Alternatively, this concentration would be expected to be exceeded approximately by 5% of the time. This is referred to as the exceedance value for exposure. It can be seen that, the smaller the concentration, the greater the degree of protection, since fewer species would be expected to be affected. Concurrently, there is a greater probability that this value will be exceeded. The level of protection can thus be selected. For instance, the probability of the concentration exceeding that below which less than 0.1% of species would be affected could be predicted. By selecting a toxicant reference concentration, the probability of a proportion of species being affected can be estimated.

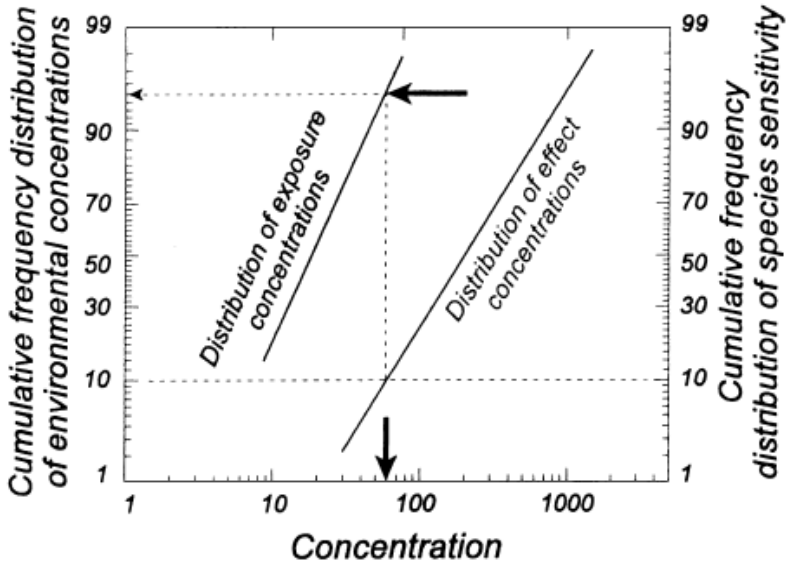


Figure 2-2 Hypothetical example of a probabilistic risk assessment showing exposure and toxicity data presented as linearized probability distributions (from Solomon et al., 2000).

PRAs are advantageous in that they make better use of data compared to deterministic risk assessments by incorporating variation in toxicity and exposures (i.e. replaces worst-case assumptions with more realistic probability distributions). Because the results of a PRA show the range of possible environmental impacts and which ones are most likely to occur, they reduce the level of uncertainty associated with a risk assessment and provide the risk manager with a flexible tool for making decisions regarding the level of certainty needed for a particular situation.

PRAs are however disadvantageous in that they are more complex and require significantly more exposure and effect data. For exposure modelling this would imply that the variability in all input parameters would need to be considered, which would result in a very large number of input parameter combinations in order to produce adequate probability distributions. This would require extensive computer processing power, leading to more time-consuming and expensive assessments. Similarly, toxicity tests covering a wide range of aquatic species would be required to generate sufficient effect data. Finally, there is no established guidance for interpreting results from a PRA. Due to their increased complexity they are generally more difficult for the public to understand and to communicate effectively.

The disadvantages described above outweigh the advantages and currently risk assessment processes for registration of pesticides rely almost exclusively on deterministic approaches.

### Tiered Risk Assessment

Given the large amount of data requirements for exposure modelling in particular, a tiered risk assessment approach is often adopted. The principle of this approach is, at the first tier, to initially perform a very simple risk assessment based on very conservative worst-case exposure input parameters (e.g. 10% of the applied quantity of a pesticide moves into an adjacent water resource) and then, if necessary, refine this process using more realistic input parameters in subsequent steps (i.e. higher tiers). The need to move to a higher tier risk assessment is dependent on the risk outcome of the initial tier. If, under the conservative conditions of the first tier, no risk is expected (i.e. RQ < 1), then there is no need to perform a risk assessment at the next highest tier using more data intensive inputs. The rationale behind this is that there is no point in performing a more detailed risk assessment if there is no risk using extreme worst-case exposure assessment data. However, if, at this first tier a risk cannot be ruled out, then a more detailed assessment takes place, using more realistic data inputs (i.e. less conservative) to perform a more realistic risk assessment. The assessment becomes more refined at higher tiers, incorporating increasingly realistic data inputs that are integrated by increasingly complex modelling approaches (e.g. environmental fate of the pesticide is considered), accounting for multiple transport routes (Figure 2-3). The EU currently makes use of an established tiered risk assessment approach for registration of pesticides.

Effect assessment can also become increasingly complex, starting from standard single species toxicity tests at lower tiers, to multispecies microcosm tests at higher tiers where ecological processes are incorporated into the experimental design.

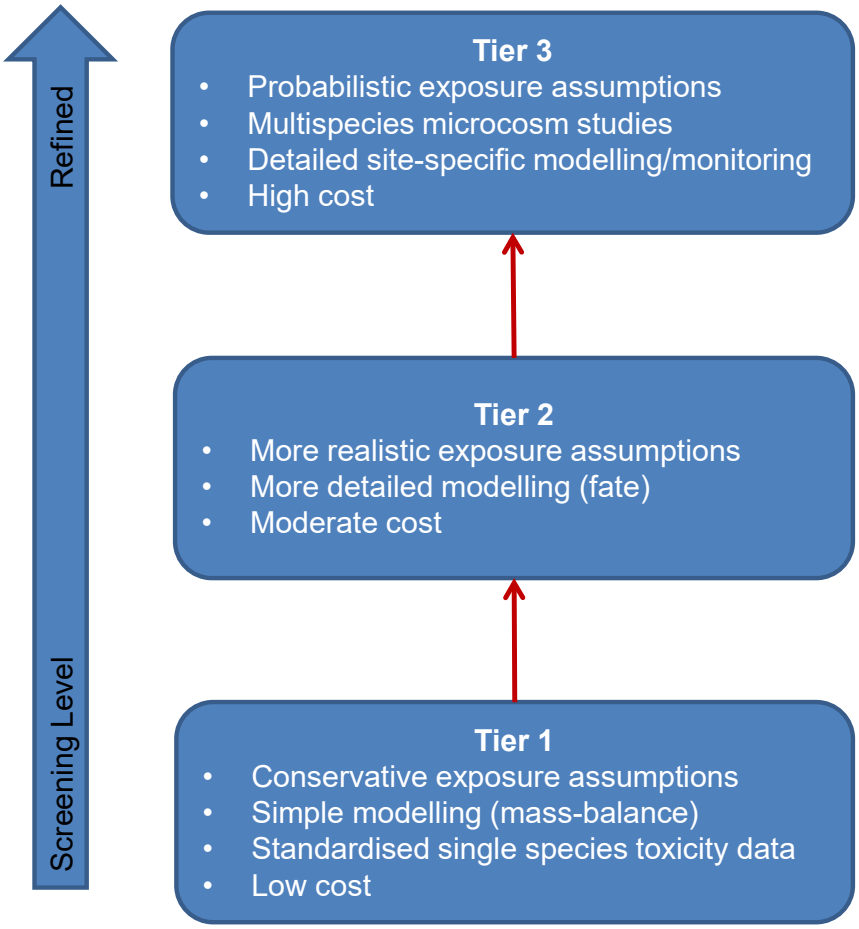


Figure 2-3 Schematic illustrating the principles of a tiered risk assessment process.

## 2.10. Pesticide Registration Protocols

### European Union

Pesticide registration in the EU is regulated according to Directive 91/414/EEC. The European Union has harmonised the conditions and procedures for authorising plant protection products so as to protect human health and the environment. It has also drawn up a list of authorised substances and a phased programme for evaluating substances already on the market. From an aquatic ecosystem perspective the main objectives of the risk assessment are to evaluate the possibility of a plant protection product (pesticide) reaching surface water under the proposed conditions of use. If this possibility exists the short- and long-term predicted concentration (PEC) of the active ingredient (and metabolites) that could be expected in the surface water in the area of envisaged use after use of the plant protection product according to the proposed conditions of use should be estimated. The risk that these PECs pose to aquatic organisms should be evaluated using relevant assessment endpoints that ensure protection of the aquatic ecosystem.

*Exposure Assessment*

Surface water exposure estimation component of the risk assessment process takes place according to a stepwise or tiered approach as illustrated in Figure 2-4 (FOCUS, 2001). These steps are often referred to as FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe) steps.

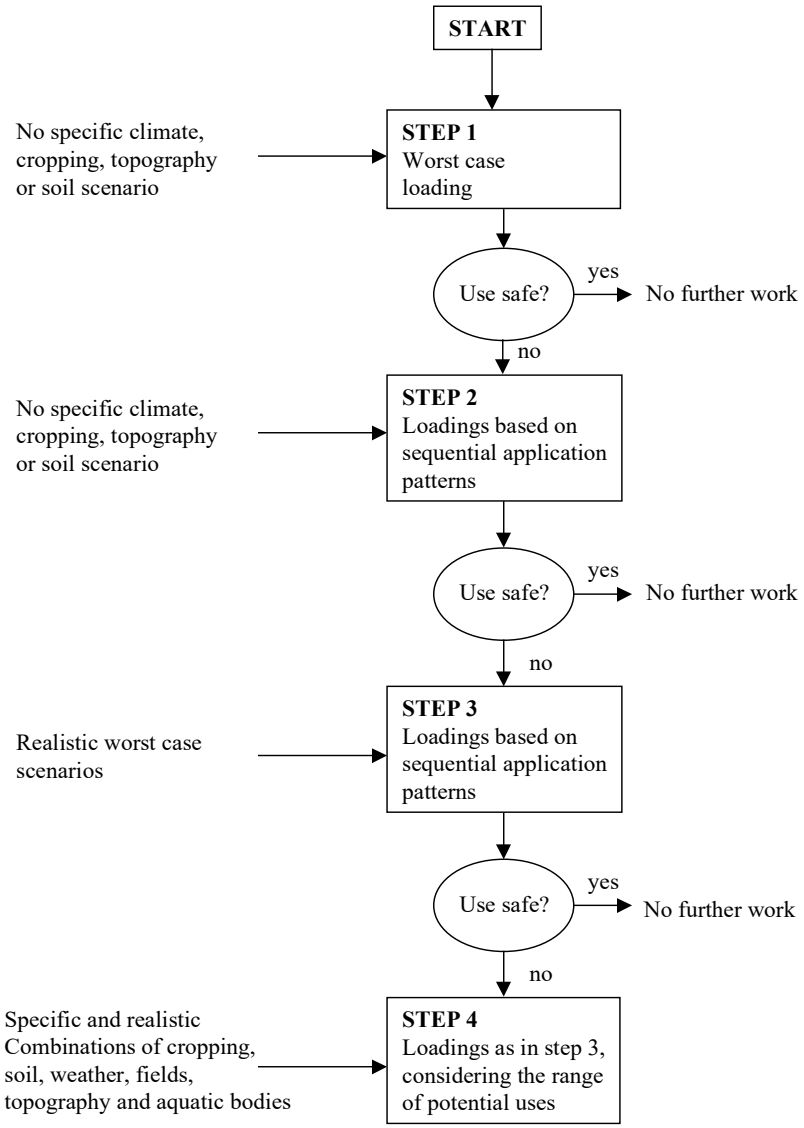


Figure 2-4 Schematic illustrating the tiered risk assessment approach adopted by Directive 91/414/EEC for the registration of pesticides in the EU (FOCUS, 2001).

The first FOCUS step in the tiered approach is to estimate surface water exposure based on an "extreme worst case loading" scenario (i.e. inputs of spray drift, runoff and drainage are evaluated as a single loading to the water-body). The estimated exposure may be compared to the relevant toxicity concentrations, the lethal or effect concentration, L(E)C50, or the No-effect concentration (NOEC), of

the water organisms investigated. If, at this early stage, the use is considered safe no further surface water risk assessment is required.

If however, the result indicates that use is not safe, it is necessary to proceed to a Step 2 exposure assessment. This step assumes surface water loading based on sequential application patterns taking into account the degradation of the substance between successive applications. A time-weighted average concentration is calculated as a result of all individual loadings. Again the PEC's are calculated and may be compared to the same and/or different toxicity levels for aquatic organisms. As with Step 1, if the use is considered safe at this stage, no further risk assessment is required whereas an 'unsafe' assessment necessitates further work using a Step 3 calculation.

In Step 3, more sophisticated modelling estimations of exposure are undertaken using a set of 10 scenarios representing 'realistic worst-case' situations for surface water within Europe. Environmental parameters (e.g. climate, topography, soil type, nature and extent of water bodies, etc.) are derived from each of these scenarios and used as input into detailed fate and transport models. These models include regression models (spray drift), MACRO (drainage), PRZM (runoff) and TOXSWA (models the fate of pesticides upon entry into the water body). At this stage, the calculated PECs for each scenario are compared with relevant toxicity data and a decision made as to whether it is necessary to proceed to Step 4 exposure estimation. Risk assessments using Step 3 exposure estimation may incorporate higher-tier toxicity data generated from micro- or mesocosm studies.

The final step of the FOCUS process is Step 4. In principle, Step 4 can be regarded as a higher-tier exposure assessment step. This may include a variety of refinement options of different degrees of complexity covering risk mitigation measures, refinement of fate input parameters, or regional and landscape-level approaches. By its nature, Step 4 is a 'case-by-case' process, depending on the properties of the compound, its use pattern, and the areas of potential concern identified in the lower tier assessments. As such, no specific recommendations have been formulated for the Step 4 process. A Step 4 analysis is only considered necessary for those applications that failed Step 3 and for which the applicant wants to continue the registration process.

*Effect Assessment*

As part of the risk assessment framework, PECs are compared to toxicity data derived from test organisms representative of the aquatic ecosystem. Daphnia, rainbow trout (*Oncorhynchus mykiss*), blue-gill sunfish (*Lepomis macrochirus*) and green algae are used as test organisms to represent aquatic invertebrates, cold fish species, warm fish species and aquatic plants, respectively (FOCUS, 2002). For invertebrates and fish, acute toxicity data are always required, and chronic data are also required if there is continued or repeated exposure to be expected (i.e. if a compound is applied more than once per season, or if the dissipation rate (DT50) in water is greater than or equal to 2 days). In practice, this means that chronic data are nearly always required. In the preliminary risk assessment,

uncertainty factors of 100 and 10 are applied to acute and chronic endpoints, respectively, to account for potential inter-species differences in invertebrate sensitivity and other sources of uncertainty. Daphnia is used as a representative invertebrate because of its ease of culture and testing, the availability of international acute and chronic guidelines (OECD 202 and 211), and its sensitivity to toxicants. For herbicides an additional test is required on another algal species from a taxonomic group to that of green algae (i.e. blue-green algae or diatom species) as well as for a higher aquatic plant (*Lemna sp.*).

Where environmental fate and behaviour data indicate that a pesticide is likely to partition to and persist in aquatic sediments, expert judgement should be used to decide whether an acute or chronic sediment toxicity test is required. In this instance *Chironomus sp*. is the recommended test organism to assess potential effects on sediment-dwelling organisms.

*Risk Determination*

As the tiered approach for surface waters indicates at each step a comparison should take place between the calculated PEC at the level under consideration and relevant ecotoxicological data. Generally, the lowest value of the acute toxicity data (LC50 or EC50) for aquatic organisms (i.e. algae, daphnia and fish) is compared to the highest PEC in surface water and the Toxicity to Exposure Ratio (TER) is calculated. The TER is the inverse of the risk quotient (RQ). Under this approach, the TER must be maintained above levels of concern (i.e. TER > 1). For the long-term assessment, the lowest no effect concentration (NOEC) for the same aquatic organisms or, if available another aquatic organism, is compared to the time-weighted average concentration over the appropriate time period. If the TER are met, it can be assumed that the given use of the active substance has no unacceptable impact on the aquatic environment and no further work for surface water is needed. If the TER-trigger is breached the risk evaluation is taken to Step 2. If the evaluation shows acceptable risk at Step 2 no further work is needed for surface water. If again the trigger is breached the process is taken forward to Step 3 and the required scenarios are calculated. From this Step 3 assessment there are several possible outcomes considering the initial, short term and long-term risk assessment considering the lowest value of the acute and chronic toxicity data of all the available taxa:

1. The calculated TER derived from estimated PEC (initial, short-term or long-term) for a substance may exceed the TER-trigger value for all relevant scenarios
2. The calculated TER derived from estimated PEC (initial, short-term or long-term) for a substance does not exceed the TER-trigger value for any relevant scenario
3. The calculated TER derived from estimated PEC (initial, short-term or long-term) for a substance may exceed the TER-trigger value for some and does not exceed the TER-trigger value for other relevant scenarios.

The following actions are proposed to be taken in the different situations:

- If the calculated TER derived from the estimation of the PEC for a substance exceeds the TER-trigger value for all relevant scenarios, then registration of the pesticide would not be possible unless convincing higher tier data (e.g. higher tier ecotoxicology studies, monitoring data, more refined modelling) are made available to demonstrate an acceptable risk to aquatic organisms. It is also possible to use Step 4 considerations, including risk management options, like buffer zones, drift reducing nozzles, etc.
- If the calculated TER derived from the estimation of the PEC for a substance does not exceed the TER-trigger values for any relevant scenario, there can be confidence that the substance can be used safely in the great majority of situations in the EU.
- If the calculated TER derived from the estimation of the PEC for a substance may exceed the TER-trigger value for some and does not exceed the TER-trigger value for other relevant scenarios, then in principle the substance can be registered for use with respect to the assessment of its possible impact on surface water bodies. The scenarios represent major agricultural areas of the EU, and, consequently, also “safe” uses are significant in terms of representing large agricultural areas in the EU. However, when making decisions in these cases, the full range of results should be evaluated with the aim to specify critical conditions of use as clearly as possible.

**United States of America**

In the USA the registration of pesticides and assessment of their human and environmental safety is the responsibility of the US Environmental Protection Agency (US EPA). The whole pesticides risk assessment process is founded on the Guidelines for Ecological Risk Assessment (USEPA, 1998a). The following sections describe what the data requirements are for the assessment of exposure and effects, and also how the obtained information is integrated for risk assessment purposes.

*Exposure Assessment*

The exposure assessment undertaken by the US EPA for pesticides risk assessment is aimed at defining an exposure profile (potential or actual contact) for a particular pesticide with aquatic biota. The generated from the exposure profile include the following information: source, recipient biota, fate and transport of the pesticide (exposure pathways), and concentration dynamics of the active ingredient or its breakdown products (concentration, frequency, duration).

The data obtained from this step should define amongst other aspects the physico-chemical transformation of the active ingredient in the recipient environment, i.e. degradation, persistency, mobility, etc. The lower tier assessment level is generally qualitative and obtained exposure profile can then be used to decide whether further exposure assessment (higher tier) is required and how the further studies need to be designed. The quantitative exposure profile is drawn from higher tier further

studies (laboratory and field based) which then provide a more real world picture of the environmental fate of the active ingredient or its breakdown product. The data required by the US EPA in this aspect (Fate and Transport) is as follows: hydrolysis, photo-degradation in air, water and soils/sediments, biological degradation, volatility (field and laboratory), leaching and absorption/adsorption, dissipation, and ground water monitoring. The probable routes and rate of pesticide flow/transport in the aquatic environment are obtained from mimicking the actual pesticide use under field conditions, whereas laboratory studies assess a single dissipation process at a time. For instance, field trials can assess spray drift in order to evaluate the extent of pesticide migration from the application site and such information can then be used to prescribe environmental conditions under which application should take place and equipment required as a measure to contain pesticide drift to non-target recipients'. To derive estimated environmental concentrations (EECs) for water resources the US EPA generally follows a tiered approach where screening models are used at lower tiers (FIRST, GENEEC) and more complex models are used at higher tiers (PRZM-EXAMS) as more robust risk assessment is needed. For all the data required the testing guidelines are provided by the US EPA.

*Effect Assessment*

The effects assessments are mostly undertaken with the active ingredient but the toxicity of breakdown products and other formulation (if known) is incorporated in the risk assessment. The effects data required is predominantly derived from laboratory studies, however where uncertainties arise from such studies, field studies may be required. The requirements are categorised into acute and chronic effects observed from dose-response relationships.

For the acute effects on invertebrates the Daphnia sp. (invertebrate model) 48 hour immobilization EC50 and mortality LC50 for are required. For the acute effects on vertebrates including amphibians, fish are used as models and the LC50s for both cold (rainbow trout) and warm (bluegill) water species are required. Fish are also usually used to investigate the pesticide's bioconcentration, bioavailability, and biomagnification potential.

The lower tier of chronic effects assessment to invertebrates focuses on the reproduction and development effects of Daphnia and Penaeid prawn, where the reported NOECs endpoints are for survival, number of hatchlings, growth and developmental rate. For vertebrates (fish), the chronic effects are investigated on early life stage and full life cycle. The early life stage effects are reported as NOECs for hatching rate, hatching time, embryo survival, time to swim-up, growth-weight and length. The full life cycle assessment focusses on survival, growth and reproduction impairment and the endpoints measured include egg production number, embryo hatching rate, hatching duration, number of surviving larvae hatched, growth-weight and length. Higher tier assessment of chronic effects can include the same endpoints but undertaken in mesocosm studies in order to ascertain if laboratory observations will differ to field observations differ, and also to investigate application under different scenarios.

Furthermore, within the US EPA scheme for effects assessment there is consideration for potential pesticide exposure of non-target plants under circumstances where the pesticide may move (drift) away from intended application site. Generally the assessment on non-target plants focuses on growth effects and reported as the EC50 and NOAEC depending on specific endpoint data requirement. Under the first tier; the effects of fungicides at the highest application rate (worst case scenario) are tested on algae (*Pseudokirchneria subcapitata*) and a higher plant (*Lemna gibba*). For herbicides the testing is also undertaken under the highest application rate and effects are assessed on *Skeletonema costatum, L. gibba, Anabaena flosaquae, P. subcapitata*, and a freshwater diatom, usually *Navicula sp*. The second tier effects assessment reports the EC50 and NOAECs of the five species used in first tier. The third tier effects assessment is undertaken in the field setup if the pesticides toxicity in lower tier resulted to greater than 50% effects on plant growth.

All the obtained effects data is then categorised depending on level of observed effects and the categories are: very highly toxic (< 0.1 mg/L), highly toxic (0.1-1 mg/L), moderately toxic (>1-10 mg/L), slightly toxic (>10-100 mg/L), and practically non-toxic if toxicity was only observable when exposure concentration was greater than 100 mg/L.

*Risk Determination*

Risk determination/characterization consists of two interlinked components namely; risk estimation and risk description. Risk estimation involves the integration of the data collected under the assessment of exposure and effects to estimate the risk, together with associated assumptions, uncertainties, weaknesses and strengths of the process. Risk description on the other hand is the interpretation of risk based on assessment endpoints where the Levels of Concern (LOC) are evaluated based on data status, level of uncertainty, and the linkage of obtained evidence to risk assessment objectives/questions.

The US EPA mostly undertakes deterministic risk approach where the effects are compared to the exposure, then calculate the risk quotient (RQ). The RQ is obtained by dividing exposure (e.g. EEC) by effects (e.g. NOAEC):

*RQ= exposure/toxicity.*

The lower tier/screening endpoints previously described are predominantly used to determine the RQ. For the algae and higher plants the RQ is calculated as:

*Acute RQ = highest exposure concentration/most sensitive organism LC50/EC50*

For invertebrates the chronic RQ is calculated as:

$$Chronic\ RQ_{invertebrates} = 21\ day\ mean\ concentration/NOAEC$$

For the vertebrates the chronic RQ is calculated as:

$$Chronic\ RQ_{fish} = 56\ or\ 60\ day\ mean\ concentration/NOAEC\ (early\ life\ stage\ or\ full\ life\ cycle)$$

For the purposes of risk description, the calculated RQs are then are then assessed against the LOCs which are set by the US EPA as means to interpret the RQ. Simply put; the LOCs are set levels/categories of risk which the RQ is interrogated/interpreted against (Table 2-3). The LOCs have built in safety factors although these are not as conservative as those used by the EU. For acute and chronic toxicity data, safety factors are 2 and 1, respectively (100 and 10 for EU), while factors of 10 and 20 are applied for restricted use and protection of endangered species.

Table 2-3 Risk presumptions for aquatic biota

| **Organism** | **Risk presumption** | **RQ** | **LOC** |
|---|---|---|---|
| Animals | Acute high risk | EEC/$LC_{50}$ or $EC_{50}$ | 0.5 |
| | Acute restricted use | EEC/$LC_{50}$ or $EC_{50}$ | 0.1 |
| | Acute endangered species | EEC/$LC_{50}$ or $EC_{50}$ | 0.05 |
| | Chronic risk | EEC/NOAEC | 1.0 |
| Plants | Acute high risk | EEC/$EC_{50}$ | 1.0 |
| | Acute endangered species | EEC/$EC_{50}$ or NOEAC | 1.0 |

For more complex/advanced risk determinations that are intended for more than screening purposes, the USE EPA has since the late 90s adopted the probabilistic risk assessment (PRA) approach to inform the Agency's decision making (US EPA, 1997). Such arises from recognition that the environment as a whole is variable and there's always going to be some level uncertainty when dealing with environmental issues, hence a need to incorporate such aspects in decision support tools. Furthermore, the PRA is applied in a tiered manner such that the uncertainty and variability assessment can be undertaken at differing levels of data intensity or availability (NRC, 2009). The advantage of PRA over the single value deterministic approach; is that PRA can be flexible to the intensity of data available thus better outline uncertainty level which can be better adopted to analyse risk for different environmental scenarios or management options. Thus the PRA produces a wide range of risk scenarios (compared to a single value) such that the decisions can be taken at varying levels of certainty and mitigation measures.

**Australia**

The Australian Pesticides and Veterinary Medicines Authority (APVMA) is tasked with the registration for use in Australia, however other State institutions do play a supportive role to APVMA. A variety of data requirements are set to applicants who wish to register pesticides or even change conditions of earlier registration. Also required for registration is the pesticide's environmental information which includes environmental fate and behaviour (exposure) as well as effects to terrestrial and aquatic biota. Collectively the information provided by the applicant is used to evaluate environmental risk that could arise from the application of the pesticide or its active ingredients.

*Exposure Assessment*

The exposure assessment component generally deals with estimating how much of the pesticide/active ingredient will remain in the environment, and this is done by considering the pesticide's application conditions, environmental entry and deposition, physico-chemical transformations, and its environmental flow. The amount is called the predicted/estimated environmental concentration (PEC/EEC). The set of data required for the exposure assessment is summarised in Table 2-4. The data relating to environmental chemistry and behaviour is required in order to characterise its persistence and mobility in the environment. The triggers for such information include the use of the pesticide, application patterns, and the known physical and chemical properties of the pesticide. Of interest are the following characteristics: physico-chemical degradation, biological degradation, mobility, bioconcentration, field dissipation, spray drift and vapour drift.

*Effect Assessment*

The effects assessment data requirements are to enable the regulators to determine the hazard posed by the pesticide/active ingredients or its break down products. For the first tier three trophic levels are tested for acute and chronic effects under the aquatic ecotoxicity scheme, namely; primary producer (algae/higher plants), primary consumer (invertebrates), and secondary consumer (fish). Higher tier testing is triggered by the observations from acute effects, pesticide use patterns and its physico-chemical as well as toxicity properties. Australia has adopted the USEPA and EU approaches for the assessment of pesticides effects to aquatic biota.

Table 2-4 Data requirements for the exposure assessment carried out as part of the risk assessment for registration of pesticides in Australia (APVMA, 2016).

| **Information requirement** | **Description** |
|---|---|
| Amount of chemical | Estimated amount to be used (tonnes or litres) |
| Manufacturing | When manufacturing and packaging is within Australia:<br>Quantity released into the environment (effluents for water) from formulation, packaging and waste management steps.<br>Manner of waste disposal during manufacturing and packaging. |
| Use and application | Application method<br>Factors influencing mobility (droplet size, equipment used) |
| Product disposal | Empty containers, unused product, dilution for use |
| Predicted environmental concentration | PECs for soil, water and air. If exposure for a particular recipient is not anticipated then applicant can apply for data waiver. |
| Tiered PECs | First tier prediction at worst case scenario, if the 1$^{st}$ tier induces toxic effects then further tier assessments consider more realistic exposure scenarios |
| $PEC_{water}$-Spray drift | First tier $PEC_{water}$ assumed direct application to a defined size water body, generating acute and chronic (if persistent) PECs. Initial tier PECs then refined to estimate spray drift exposure, which can be further refined at higher tiers under more realistic conditions. |
| $PEC_{water}$-Run-off and drainage | Exposure from run-off and drainage derived from prescribed model (Probst et al., 2005). Lower tier screening assessment overlooks chemical properties, but further tiers include such details including topography details. The initial tier screening can be used to exclude low risk chemicals such that more analytical efforts can be aimed at higher risk candidate pesticides. |
| Refined run-off PECs | Only undertaken if initial run-off screening predicted that aquatic biota may be exposed to toxic concentrations. Thus a refined assessment of edge-of-field assessment is required, including chemical and soil properties integration. The tiered assessment follows a prescribed OECD model (ANRA, 2001). |
| $PEC_{sediment}$ | For hydrophobic pesticides the $PEC_{sediment}$ can be derived from the pesticide's organic carbon partitioning coefficient (Koc) |

Primary producers: The first tier effects assessment for primary producers is undertaken with *P. subcapitata* and *L. gibba* as per the US EPA approach, at the highest application rate except for herbicides. For herbicides the number of species increases to five including *S. costatum*, *A. flos-aquae*, and *Navicula sp*., and the testing is done at the highest application rate. The second tier level of assessment is done with the five species following a dose-response manner. Both tiers focus on growth effects and report the EC50s. Following the EU effects assessment approach; testing with *P. subcapitata* is a standard requirement but for herbicides and plant growth regulators an additional algal species from a different taxonomic group is required. The endpoints reported are biomass (cell number) and growth rate. For higher plants the testing utilises *Lemna sp*., where the number of fronds is considered to be a key endpoint but other endpoints may be used where appropriate for the risk assessment.

Primary consumers: The 48 hr *Daphnia* EC50 (mortality or immobilisation) with *Daphnia* is considered a fundamental data requirement for acute effects as Tier I. If the toxicity of the chemical to

*Daphnia* is low (48 hr EC50 > 1 mg/L, 21 d NOEC>0.1 mg/L) then the *Chironomus riparius* acute water only test with first instar larvae should instead be utilised. Depending on Tier I results, the *Daphnia* reproduction test (21d NOAEC) may be needed for the second tier effects assessment.

Secondary consumers: The 96 hr LC50 for fish is considered a fundamental Tier I data requirement for acute effects. As per the US EPA approach, both the cold and warm water species are tested. Chronic effects assessment are considered to be Tier II assessment level and evaluates reproductive capability endpoints that include number of embryos hatched, time to hatch, embryo mortality, time to swim up, growth-weight and length (LC50 and NOAEC reported). The need for chronic data is based on expert judgement as there is no formal criterion, and the data may not be provided if the applicant demonstrate that continued or repeated exposure is unlikely and that the chemical is not persistent. The next level tier (III) may be necessary in to closely estimate risk in the field, and for such purposes microcosm and mesocosm studies are used. The assessment of secondary exposure effects may be considered, for instance for substances that are highly adsorptive, have log Kow ≥ 3, etc. Furthermore, secondary exposure effects may be assessed for fish eating predators

*Risk Determination*

The integration of the exposure and effects assessment outcomes in the risk evaluation step follows a deterministic approach where the risk quotient (RQ) is calculated as the primary end result. The RQ is then is compared with levels of concern in or order to either conclude risk as acceptable/not, or further testing required, or recommend risk mitigation measures so as to reduce the risk to acceptable levels. Accompanying the RQ should be the description of associated uncertainties, assumptions, strengths and limitations. The acute RQ is calculated as PECwater/LC or EC50 (most sensitive organism), whereas for the chronic scenario it is PECwater/NOEC (most sensitive organism). The RQs are then compared to LOCs in order to assess potential risk to non-target organisms:

*RQ > 0.5 = unacceptable risk (for acute toxicity data)*
*0.1 ≤ RQ ≤ 0.5 = risk may be mitigated by controlled use (for acute toxicity data);*
*RQ < 0.1 = low risk potential (for acute toxicity data);*
*RQ < 1 = risk considered acceptable (for chronic toxicity data).*

In cases where the RQ exceeds the level of concern, a higher risk assessment must be performed. Such can be undertaken through refinement of exposure and effects assessment steps, for instance through advanced modelling or chemical analysis or undertaking microcosm or mesocosm studies.

## 2.11. How Protective are Risk Assessments?

Although detailed risk assessments are required before pesticides are registered for use, very few studies have actually compared the outcome of environmental risk assessments (i.e. concentrations that are protective of the aquatic ecosystem) to monitoring data collected in the field under normal agricultural practices. Stehle et al. (2015) conducted a comprehensive meta-analysis using peer-reviewed literature on agricultural insecticide concentrations in EU surface waters and evaluated associated risks using Regulatory Acceptable Concentrations (RACs – final toxicity value derived as part of the effect assessment) obtained from official European pesticide registration documents. In 44.7% of 1566 cases, measured insecticide concentrations (MICs) in EU surface waters exceeded their respective RACs. The authors concluded that in spite of the rigorous risk assessment process followed, current EU pesticide regulations do not protect the aquatic environment and that insecticides threaten aquatic biodiversity. It is important to note however that in the EU, RACs are derived using assessment factors that could possibly be over protective. Therefore while RACs may be regularly exceeded it is uncertain as to whether MICs do in fact threaten aquatic biodiversity. RAC exceedances were significantly higher for insecticides authorized using conservative tier-I RACs and for more recently developed insecticide classes (i.e. pyrethroids). In addition, higher risks were identified for smaller surface waters that are specifically considered in the regulatory risk assessment schemes.

Studies by Knäbel et al. (2013) compared a larger data set of 122 MICs obtained from 22 field studies, to respective PECs determined using steps 1 to 4 of the EU FOCUS exposure assessment approach (FOCUS, 2001). While FOCUS step 1 and 2 PECs generally over predicted the MICs (as would be expected given the extreme worst-case nature of these exposure assessments), 23% and 31% of step 3 and 4 standard PECs, respectively, were exceeded by surface water MICs, which questions the protectiveness of the FOCUS exposure assessment. Using realistic input parameters, step 3 simulations under predicted MICs in surface water and sediment by 43% and 78%, respectively, indicating that a higher degree of realism further reduced the protectiveness of model results. Similar results were obtained for a study on fungicides (Knäbel et al., 2012).

The main conclusion derived from these studies is that the FOCUS modelling approach is not protective for insecticide and fungicide concentrations in the field. Possible reasons for the discrepancy between modelled and monitored results include:

- Size of the agricultural catchment contributing to the calculation PECs is most likely under-estimated in most instances.
- Timing of simulated rainfall events in relation to the application of a pesticide has a significant influence on runoff derived pesticide concentrations and this may not be accurately accounted for in modelling predictions.
- Inherent variability in physicochemical properties used in exposure modelling (e.g. Koc and DT50 of pesticides)

- Standard daily runoff fluxes calculated by the runoff model (PRZM) are translated to hourly data by assuming a peak runoff rate of 2 mm/h. For example a 16 mm daily runoff event translates into an eight hour runoff loading of 2 mm/h (FOCUS, 2001). However, in reality, a large proportion of the 16 mm daily runoff occurs in a considerably shorter time period during heavy rainfall events, resulting in significantly higher in-stream concentrations.

## 2.12. Summary

- Deterministic approaches are favoured for assessing in registration of pesticides – mainly due to their relative simplicity and the ease with which results can be communicated. Probabilistic methods, while more desirable in terms of reducing uncertainty related to risk calculations, are regarded as being too data intensive.
- It is widely accepted that environmental fate parameters for pesticides vary considerably, even at small spatial scales (i.e. within a single agricultural field). Nevertheless one data point per input parameter is used for the purposes of deterministic risk assessment.
- It is recognised that due to the high variability of input parameters, the results of deterministic risk assessments are inherently uncertain.
- Worst-case scenarios are used in exposure assessment and assessment factors are applied to toxicity endpoints with the aim of executing a conservative risk assessment that ensures protection of the aquatic ecosystem.
- Different assessment (or safety factors) are employed by different regulating authorities (Table 2-5):

Table 2-5 Risk quotients and associated assessment factors used for interpreting deterministic risk assessments for pesticide registration in the EU (converted from inverse TER values), United States and Australia.

| Risk Category | Risk Quotient – (LOCs) | | | Equivalent Assessment Factors | | |
|---|---|---|---|---|---|---|
| | EU | USEPA | Australia | EU | USEPA | Australia |
| Acute High Risk | 0.01 | 0.5 | 0.1 | 100 | 2 | 10 |
| Acute Restricted Use | | 0.1 | | | 10 | |
| Acute Endangered Risk | | 0.05 | | | 20 | |
| Chronic Risk | 0.1 | 1 | 1 | 10 | 1 | 1 |

- Environmental fate data, an essential input into exposure modelling is also requested by the DAFF.
- The main hindrance in performing a more detailed risk assessment for registration of pesticides in South Africa is with regards to the exposure assessment. No exposure scenarios representative of typical worst-case agro-hydrological conditions have been defined for South Africa and no environmental fate models are used to predict estimated environmental concentrations for the purposes of risk.
- Risks of pesticides to the aquatic ecosystem are therefore not presently accounted for during registration of pesticides in South Africa. However based on the data requested by the DAFF and depending on the availability of environmental data and suitability of models required for exposure modelling, it should be possible to perform deterministic risk assessments for pesticide registration in South Africa. This potential will be evaluated in ongoing research in this project.
- In spite of the protective nature of risk assessments employed for pesticide registration, research conducted in the EU has shown that in spite of this rigorous approach, pesticide concentrations measured in the field frequently exceed worst-case derived PECs and RACs. It would therefore appear that using worst-case scenarios in exposure assessment does not always satisfy the main objective of the risk assessment.

# 3. Evaluation of Deterministic Models

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## 3.1. Background

Pesticides enter surface waters through runoff, spray drift, and deposition. Once pesticides have entered surface waters, they are exposed to a number of physical, chemical, and microbial processes that influence the fate of the pesticide in the way body. These processes include photodegradation, volatilization, biodegradation, absorption/adsorption, chemical degradation, leaching, and sedimentation. Aquatic exposure assessments typically rely on mathematical models that capture these processes and predict the concentration of pesticides in surface waters.

Predicted Environmental Concentrations (PECs) are calculated using laboratory generated environmental fate data that describe how fast the pesticide breaks down in the environment and how mobile it is in the environment. In South Africa this data is typically supplied by an applicant seeking to register a product for agricultural use, yet the registering authority does not make use of any exposure models to predict how the pesticide will behave in the environment. Modelling provides an indirect estimate of pesticide concentrations and can estimate concentrations continuously over long periods of time and for vulnerable areas of interest. Modelling forms an important part of the exposure assessment and PECs are compared with toxicity data (generated in the effect assessment) to determine the risk a pesticide poses to the aquatic ecosystem. Models can also be used to determine how various mitigation practices affect the amount of the pesticide that enter water resources and reduce risk to aquatic biota.

As highlighted in the literature review, regulators typically apply a tiered approach in estimating PECs. The intent of this approach is to estimate PECs in water from sites that are highly vulnerable to spray drift, runoff or leaching. With this approach, pesticides that pass the first tier (i.e. the PEC does not exceed the toxicity endpoint concentration) will likely pose a low risk to the aquatic environment. Failing a tier, however, does not necessarily mean the chemical is likely to cause health or environmental problems, but rather that there is a need to move to a higher tier and conduct a more refined assessment. Lower tier assessments typically use very simple, conservative mass balance modelling approaches (environmental fate is not considered), while higher tier assessment will utilise more realistic, complex models that consider the fate of the pesticide in the environment (i.e. time taken to break down, adsorption, etc.) and the dynamics of the surface water ecosystem. A tiered modelling system is designed to provide a thorough analysis of each pesticide, while at the same time focussing more detailed efforts on those pesticides that pose the greatest potential risk.

## 3.2. Lower Tier Models

### USEPA (GENEEC 2)

In the past the USEPA used GENEEC2 as a Tier I screening model for assessing exposure of aquatic organisms and the environment to pesticides. GENEEC2 provides a rapid screen to separate the low risk pesticides from those that need more refined assessments. The model estimates high level exposure values of pesticides in surface water from a few basic chemical characteristics and pesticide label use and application information.

GENEEC2 considers adsorption of the pesticide to soil or sediment, incorporation of the pesticide at application, direct deposition of spray drift into the water body, and degradation of the pesticide in soil before runoff and within the water body. It is a single-event model, meaning that it assumes one single large rainfall/runoff event, which occurs on a 10-hectare field and which removes a large quantity of pesticide at one time from the field to a pond. In this case, the pond has a 20 000 $m^3$ volume and is 2 meters deep. The GENEEC2 program is generic in that it does not consider differences in climate, soils, topography or crop in estimating potential pesticide exposure.

GENEEC2 is expected to overestimate pesticide concentrations in surface water for most sites and may be inappropriate for some chemicals, especially those that are persistent and/or have a high sorption coefficient, as well as frequently applied pesticides. In these cases, users should go directly to a higher tiered assessment using the more sophisticated Surface Water Concentration Calculator discussed below.

GENEEC2 is no longer supported by the USEPA and at the time of writing it is not clear whether the USEPA still uses a screening model in their risk assessment approach and the identity this model.

### European Union (Step 1 Modelling Approach)

At Step 1 (or Tier 1) inputs of spray drift, run-off, erosion and/or drainage are evaluated as a single loading to the water body and “worst-case” surface water and sediment concentrations are calculated. The loading to surface water is based upon the number of applications multiplied by the maximum single use rate – unless 3 x DT50 in sediment/water systems (combined water + sediment) is less than the time between individual applications. In such a case the maximum individual application rate is used to derive the maximum PEC as there is no potential for accumulation in the sediment/water system. For first order kinetics the value of 3 x DT50 is comparable to the DT90 value.

*Runoff Loadings*

At Step 1 the run-off/erosion/drainage loading to the water body is set at 10% of the application (a very conservative estimate for the loading). The runoff/erosion/drainage entry is distributed instantaneously between water and sediment at the time of loading according to the Koc of the compound. In this way compounds of high Koc are added directly to the sediment whereas compounds of low Koc are added to the water column in the 'run-off/drainage' water.

**European Union (Step 2 Modelling Approach)**

Step 2 is a higher tier approach, but is still relatively simple. At Step 2 inputs of spray drift, run-off, erosion and/or drainage are evaluated as a series of individual loadings comprising drift events (number, interval between applications and rates of application as defined in Step 1) followed by a loading representing a run-off, erosion and/or drainage event four days after the final application. This assumption is similar to that of the GENEEC model used by the USEPA. Degradation is assumed to follow first-order kinetics in soil, surface water and sediment and the registrant also has the option of using different degradation rates in surface water and sediment.

**OECD Risk Indicator Model**

The OECD as part of their development of a pesticide risk indicator for both human health and the environment developed a simple model designed to estimate the percentage of an applied pesticide that leaves an agricultural field as runoff following a rainfall event (OECD, 1998). The equation essentially consists of empirical and physical components, including a hydrological model predicting runoff amounts, catchment related factors which influence the extent of runoff, a first-order kinetic model describing the degradation of a pesticide and a term referring to the proportion of pesticide occurring in the water phase of runoff.

The equation is as follows:

$$L\%_{runoff} = \left( Q/P \right) \times f \times \exp\left( -t \times \ln 2 / DT50_{soil} \right) \times 100 / \left( 1 + Kd \right)$$

where:

$L\%_{runoff}$ = percentage of application dose being available in runoff water as a dissolved substance;

Q = runoff amount (mm) calculated according to hydrological models (Lutz (1984) and Maniak (1992));

P = precipitation amount (mm);

$DT50_{soil}$ = half-life of active ingredient in soil (d);

f = f1 x f2·x f3, the correction factor reflecting the influence of slope (f1 = 0.02153 x slope + 0.001423 x slope2), plant interception (PI), the percentage of applied pesticide intercepted by trees in the orchards (f2 = 1 - PI/100), and buffer width (f3 = 0.83WBZ, and WBZ is the width of buffer zone [m]; if the buffer zone is not densely covered with plants, the width is set to zero);

t = time (d) between application and rainfall;

Kd = (Koc x %OC), a factor reflecting the tendency of the pesticide to bind to organic carbon in the soil, where Koc is the sorption coefficient of the active ingredient to organic carbon (mL/g) and OC% is the organic carbon content of the soil.

Tables developed by Lutz (1984) and Maniak (1992) are used to obtain the Q value corresponding to rainfall events above 10 mm. The methodology used to derive Q in this equation is relevant to German conditions. Other approaches could be used to estimate runoff amounts (e.g. the Soil Conservation Service Curve Number approach). While this is a relatively simple model, the Australian Pesticides and Veterinary Medicines Authority (APVMA) use this model for registration of pesticides in Australia (Lee-Steere, 2007).

*Application of OECD Model in South Africa*

The OECD model has been rigorously tested in the Lourens River catchment, Western Cape, South Africa. Dabrowski and Schulz (2002) used the model to estimate loadings and PECs of azinphos-methyl in the mainstem and tributaries of the Lourens River. PECs corresponded well with measured concentrations taken during monitored runoff events and demonstrates the potential of the model for use in risk assessment for registration purposes.

An additional study conducted in the Lourens River catchment used the equation as an indicator to predict the relative mobility and occurrence of several pesticides in the river following runoff events (Dabrowski and Balderacchi, 2013). Samples were collected weekly at five sites from the beginning of the spraying season (October) till the beginning of the rainy season (April) and were semi-quantitatively analysed for relevant pesticides applied according to the local farmers spraying programme. A comparison to monitoring data showed that the OECD model successfully identified hotspot sites and gave a reasonable estimation of the relative contamination potential of different pesticides at a site. In contrast to the previous study, the aim of this study was not to estimate PECs but rather to provide a relative indication of exposure and associated risk. In this context the model proved to be a reliable screening tool and could therefore be applicable in a lower tier assessment.

Another study conducted in the Lourens River catchment examined the effect of erosion rills on the efficiency of vegetative buffer strips (Stehle et al., 2016). The results showed that erosion rills are common in buffer strips adjacent to tributaries and represent concentrated entry pathways of pesticide runoff into the tributaries during rainfall events. Exposure modelling using the OECD runoff equation showed that measured pesticide surface water concentrations correlated significantly with runoff

losses predicted by model scenarios in which buffer strip width was set to zero at sites with erosion rills. In contrast, no relationship between predicted runoff losses and in-stream pesticide concentrations were detected in the model scenario that neglected erosion rills and thus assumed efficient buffer strips. Application of the OECD model in this context was able to show that erosion rills may substantially reduce buffer strip pesticide retention efficacies during runoff events. This suggests that the capability of buffer strips as a risk mitigation tool for runoff is largely overestimated in current regulatory risk assessment procedures conducted for pesticide authorization.

## 3.3. Higher Tier Runoff Modelling Approaches

As modelling at higher tiers relies on significant amounts of environmental data, scenarios representing typical agricultural conditions are often developed from which typical input parameters are obtained for input into the model. These scenarios are often specifically chosen to represent worst-case scenarios such that the model outcomes are relatively conservative and would automatically offer protection for areas that would not be regarded as worst-case. In order to develop the scenarios it is important to identify input parameters required by the model and the sensitivity of the model to these input parameters. The sensitivity analysis is important for identifying those input parameters for which the most reliable information possible needs to be obtained.

#### The Pesticide Root Zone Model (PRZM)

The Pesticide Root Zone Model (PRZM) is widely used by a number of regulatory authorities (e.g. United States, Canada, European Union, Australia) and has been regularly updated over time (currently in its fifth version). PRZM5 is a process model that estimates what happens to a pesticide in a farmer's field on a day-to-day basis (Young and Fry, 2016). It considers factors such as rainfall and evapotranspiration as well as how and when the pesticide is applied. It has two major components: hydrology and chemical transport.

The hydrologic component for calculating runoff and erosion of soil is based on the Soil Conservation Service (SCS) curve number technique and the Universal Soil Loss Equation (USLE) (NRCS, 2003; Wischmeier and Smith, 1978). This approach is widely used in a number of other hydrological models, including the Soil Water Assessment Tool (SWAT – Neitsch et al., 2005) and the ACRU model developed in South Africa (Schulze, 1989). Evapotranspiration of water is estimated from pan evaporation data. Total evapotranspiration of water includes evaporation from crop interception, evaporation from soil, and transpiration by the crop. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point, and curve number.

The chemical transport component simulates pesticide application on the soil or on the plant foliage. Dissolved, sorbed, and vapor-phase concentrations in the soil are estimated by considering surface

runoff, erosion, degradation, volatilization, foliar washoff, advection, dispersion, retardation, among others.

PRZM5 caters for the input of environmental exposure scenarios that represent a unique combination of climatic conditions, crop specific management practices, soil specific properties, site specific hydrology, and pesticide specific application and dissipation processes. Each simulation is conducted using multiple years of rainfall data to cover year-to-year variability in runoff. Daily edge-of-field loadings of pesticides dissolved in runoff waters and sorbed to sediment, as predicted by PRZM5, are discharged into a water body (the parameters and dimensions of which can be specified) simulated by the Variable Volume Water Model (VVWM). A summary of the model processes are provided in Table 3-1.

The VVWM simulates the processes that occur in the water body by using the runoff and spray drift loading generated by PRZM5 to estimate the fate, persistence, and concentration of a pesticide in a water body on a day-to-day basis. As such, the model accounts for volatilization, sorption, hydrolysis, biodegradation, and photolysis of the pesticide. The VVWM has the ability to vary its volume on a daily scale and to include sediment burial although these features are only used for higher tiered assessments.

Multiple year pesticide concentrations in the water column are calculated from the simulations as the annual daily peak, maximum annual 96-hour average, maximum annual 21-day average, maximum annual 60-day average, and annual average. These outputs can be compared against ecotoxicological data endpoints in order to determine risk.

Data requirements for PRZM5 are summarised in Table 3-2 and include weather, soil, field management, cropping and physicochemical data. Relevant sources of data for applying the model in South Africa are also provided in Table 3-2. In summary all data required as input into the PRZM5 model is available in South Africa, the sources of which are discussed in more detail in the sections below.

*Weather Data*

ARC: The ARC-ISCW Agro-meteorology Programme maintains an operational national agro-climate network of weather stations (approximately 500) and a climate databank. Hourly, daily, monthly, yearly or long-term average data is available for all parameters required by PRZM5.

Weather SA: The South African Weather Service is an additional source of information of relevant weather data. The cost of procuring the data is however quite expensive.

Table 3-1 Summary of process modelled in PRZM5

| Model | Aspects Considered | Description |
|---|---|---|
| Hydrology Model | Spatial Distribution | Homogenous |
| | Infiltration Model | Capacity model |
| | Evapotranspiratio n Model | Estimated using daily temperature and solar radiation data using the Penman-Monteith approach or using pan evaporation data with appropriate correction factor. |
| | Capillary Rise | Not considered |
| | Runoff Model | USDA SCS Curve Number |
| | Preferential Flow | Not considered |
| Erosion Model | Spatial Distribution | Homogenous |
| | Soil Erosion | MUSLE |
| | Particle Transport Model | The model calculates a peak runoff rate using a trapezoidal hydrograph and a user input storm duration. An enrichment factor is then calculated using an empirical approach. |
| | Agronomy Model | Cropping and management parameters can be modified to influence the erosion model as rotation occurs. |
| Pesticide Model | No. of Molecules | Up to three (including metabolites) |
| | Metabolites | Up to two with one parent molecule |
| | Sorption | Linear sorption based on Kd. Dependency on environmental parameter. User can specify Kd for each depth horizon or enter the Koc along with organic carbon for each depth horizon. |
| | Degradation in soil | First Order Kinetec |
| | Dependency on environmental parameters | No correction for temperature or soil moisture content. Decay rate can vary with depth. |
| | Mechanisms Considered | Hydrolysis, volatilization, microbial degradation |
| | Compartments Considered | Generally described as a lumped degradation rate. If data are available then sorbed, soil water and vapour phase degradation may be entered separately. Also microbial degradation can be modelled |
| | Dispersion in Soil | Dispersion and diffusion on vapour phase described using Fick's law. |
| | Dispersion in Concentrated Runoff | Concentration in the water above the surface layer is assumed to be equal to the dissolved concentration of the pesticide in the surface soil layer. |
| | Volatilization | Volatilization loss simulated using Jury's boundary layer model. |
| | Plant Uptake | Uptake is linked to the transpiration rate and can be adjusted by user. |
| | Degradation on plant surfaces | Lumped first order degradation constant (note that volatilization from leaf surface is calculated elsewhere). |
| | Foliar washoff | A foliar extraction coefficient is supplied by user (% washoff per cm of rainfall) |
| | Runoff and erosion | Mass balance approach based on results from hydrology and erosion sub-models. The model uses the fine enrichment factor calculated by the erosion model to calculate pesticide concentration on eroded soil particles. The water layer directly in contact with the surface soil is assumed to have the same concentration as the soil pore water in the uppermost soil layer. |
| | Cultivation | No |
| | Irrigation | Furrow irrigation, flood irrigation, and over and under canopy sprinklers are simulated. The programme has the ability to automatically trigger irrigation due to a drop in the soil water content. The time window for irrigation is set by the user. |
| | Application frequency | Multiple Applications for up to three pesticide |
| | Foliar application | Yes |
| | Soil surface application | Yes |
| | Incorporated in soil application | Yes |
| Plant Model | Foliage | Partition of foliar application between soil and foliage, volatilization and degradation can occur on the leaf surface |
| | Rooting depth | Used for hydrology and plant uptake model |

| Model | Aspects Considered | Description |
|---|---|---|
| Heat Model | | Soil temperatures are simulated and are used to correct the Henry's Law constant for temperature effects. |

Table 3-2 Data requirements and sources of data for running the PRZM5 model in South Africa.

| Date Type | Data Requirement | Data Source |
|---|---|---|
| Weather Data | Daily Rainfall | ARC/SAPWAT/WeatherSA |
| | Daily Humidity | ARC/SAPWAT/WeatherSA |
| | Daily T | ARC/SAPWAT/WeatherSA |
| | Daily T Variation | ARC/SAPWAT/WeatherSA |
| | Average Storm Duration | ARC/SAPWAT/WeatherSA |
| | Daily Solar Radiation | ARC/SAPWAT/WeatherSA |
| | Daily Pan Evaporation | ARC/SAPWAT/WeatherSA |
| | Daily Wind Speed | ARC/SAPWAT/WeatherSA |
| Soil Data | Soil Type | ARC/WR90 |
| | Core Depth | ARC/WR90 |
| | Bulk Density | SA Atlas of Climatology and Agrohydrology |
| | Soil Texture | ARC/WR90 |
| | Field Capacity | SA Atlas of Climatology and Agrohydrology |
| | Wilting Point | SA Atlas of Climatology and Agrohydrology |
| | Organic Carbon | ARC |
| Field Management Data | Field Slope | DEM |
| | Soil Erodibility | ARC |
| | Cropping Practice Factor | ACRU Manual |
| | Runoff Curve Numbers | ACRU Manual |
| | Cover Management Factors | ACRU Manual |
| Cropping Data | Emergence Date | SAPWAT 3 |
| | Maturation Date | SAPWAT 3 |
| | Harvest Date | SAPWAT 3 |
| | Max. Interception Rate (Water) | |
| | Max. Interception Rate (Pesticide) | Linders et al. (2000) |
| | Canopy Coverage | SAPWAT 3 |
| | Rooting Depth | ACRU Manual |
| Physicochemical Data | Soil/Pesticide Sorption coefficient | DAFF |
| | Decay Rate | DAFF |
| | Dissolved decay rate | DAFF |
| | Adsorbed decay rate | DAFF |
| | Vapour phase decay rate | DAFF |
| | Henry's Law coeffcient | DAFF |
| | Diffusion coefficient | DAFF |

SAPWAT: SAPWAT is a computer programme (the development of which was funded by the Water Research Commission) that is used for estimating irrigation water requirements of crops, farms and bigger areas for the planning and management of crop and area irrigation water requirements (Van Heerden et al., 2008). Irrigation requirements are estimated based on the rate of crop evapotranspiration for crops produced in a climatic region of South Africa. The model uses the internationally accepted Penman-Monteith approach for calculating reference evapotranspiration and is therefore aligned to the approach used in PRZM. It is based on the FAO 1998 Irrigation and Drainage Paper 56 “Crop Evapotranspiration” (Allen et al., 1998). Weather data and crop data are required for estimating evapotranspiration and to this end the SAPWAT software contains 50 years of derived daily weather data for each quaternary drainage region of South Africa. This database was developed from the South African Atlas of Climatology and Agrohydrology (Schulze, 2007). The derived weather stations are located at

the centroid of the polygon that represents each quaternary catchment in South Africa, providing 50 years of historical (1950-2000) daily weather data for each catchment. The weather data for each station matches that required as input for the PRZM model.

*Soil Data*

ARC: The national land type survey is the source of information of generalized soil maps of the country (Table 3-3). Broad soil patterns were organised, mainly on the basis of pedogenesis and land use capability, into 19 generalized soil patterns, organized into nine soil groups.

**Table 3-3:** Generalized soil categories for South Africa as developed by the ARC

| | |
|---|---|
| Red-yellow well drained soils generally lacking a strong texture contrast | |
| FR | Red and yellow soils with a humic horizon |
| AC | Red and yellow, massive or weakly structured soils with low to medium base status |
| CM | Red, massive or weakly structured soils with high base status |
| Soils with a plinthic catena | |
| PT1 | Red, yellow and greyish soils with low to medium base status |
| PT2 | Red, yellow and greyish soils with high base status |
| Soils with a strong texture contrast | |
| LV1 | Soils with a marked clay accumulation, strongly structured and a reddish colour |
| LV2 | Soils with a marked clay accumulation, strongly structured and a non-reddish colour. In addition one or more of vertic, melanic and plinthic soils may be present |
| Well structured soils generally with a high clay content | |
| VR | Dark coloured, strongly structured soils dominated by cracking and swelling clays (vertic soils). In addition, one or more of melanic and red structured soils may be present |
| PH/KS | Soils with dark coloured, well structured topsoil with high base status (melanic soils). In addition, one or more of vertic and red structured soils may be present |
| NT | Deep, well drained, dark reddish soils having a pronounced shiny, strong blocky structure (nutty), usually fine (red structured soils). In addition, one or more of vertic and melanic soils may be present |
| Soils with limited pedological development | |
| LP1 | Soils with minimal development, usually shallow on hard or weathering rock, with or without intermittent diverse soils. Lime rare or absent in the landscape |
| LP2 | Soils with minimal development, usually shallow on hard or weathering rock, with or without intermittent diverse soils. Lime generally present in part or most of the landscape |
| FL | Soils with negligible to weak profile development, usually occurring on deep deposits |
| Sandy soils | |
| AR1 | Red, excessively drained sandy soils with high base status – dunes are present |
| AR2 | Red and yellow, sandy well drained soils with high base status |
| AR3 | Greyish, sandy excessively drained soils |
| Strongly saline soils | |
| SC | Strongly saline soils generally occurring in deep deposits on flat lands |
| Podzolic soils | |
| PZ | Soils with a sandy texture, leached and with sub-surface accumulation of organic matter and aluminium with or without iron oxides, either deep or on hard or weathering rock |
| Rocky Areas | |
| R | Rock with limited soils |

The generalized soil map is available as a GIS layer displaying polygons of soil patterns that contain the following associated information:

- Generalised soil pattern
- Description of depth category (shallow, moderately deep or deep).
- Depth category (mm)
- Soil texture
- Clay percentage
- Leaching potential
- Rock percentage
- Description of generalised soil pattern.

*WR90*

The 1990 Surface Water Resources of South Africa Study (WR90) and its predecessors have played a major role in providing key hydrological information to water resource managers, planners, designers, researchers and decision makers throughout South Africa. Data produced as part of this study is extensive and includes a soil classification map for South Africa. The soil coverage is based on the 1989 Revised Broad Homogeneous Natural Regions map produced by the Department of Agricultural Engineering, University of Natal, Pietermaritzburg. This map categorises soils according to the binomial (or two category) classification system for South Africa (Macvicar et al., 1977). While more recent versions of the WR90 study are available (i.e. WR2005 and WR 2012), both of these updated versions still make use of the soil coverage generated for the WR90 study.

The WR90 soil data is available as a GIS layer displaying polygons of soil classification and the following associated data fields:

- Average soil depth (mm);
- WR90 soil classification;
- dominant soil series;
- the name of the dominant series,
- percentage  of the name of the dominant series,
- dominant soil texture,
- dominant series texture,
- percentage of dominant series texture;
- highest point;
- lowest elevation;
- range of elevation; and
- broad SIRI soil mapping units.

The main advantage of using the WR90 soil data is that runoff curve numbers have been generated for each of the soil classes. Runoff curve numbers are required for estimating the quantity of runoff following rainfall – an important input parameter for the PRZM model. For this reason, the WR90 soil classification is recommended for parameterising the PRZM model.

*South African Atlas of Climatology and Agrohydrology*

The SA Atlas of Climatology and Agrohydrology contains detailed maps (and associated shapefiles), at a regional level, of climatic parameters that influence the available water on agricultural potential and on agricultural sustainability for application in resource planning, primarily in the water and agriculture sectors (Schulze, 2007). The Atlas is intended as a functional user document to provide the "big picture" in South Africa, but in sufficient detail to be useful in regional and local decision making. In developing regional datasets, one of the methodologies used was to relate climate parameters which are measured at relatively few irregular point locations throughout the country (e.g. rainfall, temperature, solar radiation, vapour pressure), to known physiographically related variables such as altitude, latitude, longitude, distance from the ocean or topographic exposure, and then to apply these relationships to mapping climate parameters where no measurements are made. The Atlas synthesises over 25 years of experience with climate database development and agrohydrological modelling and is an important source of information with regards to parameterising the PRZM model, particularly with respect to information pertaining to soil characteristics (field capacity, wilting point, bulk density – Schulze, 2007) and climate (e.g. evaporation – Schulze and Maharai, 2007).

*ACRU*

ACRU is a agrohydrological multi-purpose model which integrates the various water budgeting and runoff producing components of the terrestrial hydrological system with risk analysis, and can be applied in design hydrology, crop yield modelling, reservoir yield simulation, irrigation water demand/supply, water resources assessment, planning optimum water resource utilisation and resolving conflicting demands on water resources (Smithers and Schulze, 1995).

ACRU simulates runoff volumes from the land surface using the same methodology as used in the PRZM5 model (i.e. the SCS curve method developed by the USDA). As part of the development of the ACRU model specific curve numbers were developed for different combinations of land use and soil type in South Africa. The ACRU manual provides a table of hydrological categories (defined by SCS grouping) for each soil form and series as well as a table of SCS curve numbers for crop type and associated hydrological category (dependent on soil form and series). The soil classification system used to define soils is the binomial classification system displayed in the WR90 soil coverage. As mentioned in section 1.3.4.2, the WR90 soil coverage is therefore recommended as the primary source of soil data for parameterising the PRZM model.

*SAPWAT*

Most of the cropping data required for parameterising the PRZM model is available in the SAPWAT software package. As part of the SAPWAT model typical planting, emergence, maturation and harvest dates for different crops produced in South Africa are provided. These dates are adjusted depending on the general climate of the catchment the crops are produced in (e.g. dry and hot or mild, humid, warm summers, etc.). In addition the programme estimates effective canopy cover for different crops based on estimates of percentage cover (as seen from directly above), foliage height, row width and row direction.

*Other Sources*

Interception of an applied pesticide by the target crop is an important aspect of exposure assessment as this determines what fraction of the applied substance remains on the leaves and stems of the plant and what fraction reaches the soil surface. No data for foliar interception by crops in South Africa exists. This aspect has however been examined in detail in other countries. Linders et al. (2007) published growth-phase specific interception factors for a number of crops for the purposes of performing exposure assessments in risk assessment. The factors are based on measured data for a number of crops throughout Europe and North America.

## 3.4. Higher Tier Spray Drift Models

**AgDisp**

The AGricultural DISPersal (AGDISP™) (version 8.26) is a "first-principles" science-based model that predicts spray drift from application sites. The model was developed by the USDA Forest Service. AGDISPTM was designed to optimize agricultural spraying operations and has detailed algorithms for characterizing the release, dispersion, and deposition over and downwind of the application area. This model can be used in estimating downwind deposition of spray drift from aerial and ground boom applications. In addition, it can be used in estimating downwind deposition of spray drift from forestry and adulticide/mosquitocide applications.

**AgDrift**

AgDRIFT® (version 2.1.1), a modified version of the AGDISP model, was developed as result of a collaborative effort between the USEPA, the USDA Forest Service, and the Spray Drift Task Force (SDTF). Spray drift studies conducted by the SDTF in the United States evaluated the effects of application, meteorological and tank mix variables on spray drift (Hewitt et al., 2002). The data from these studies have been incorporated into AgDRIFT, the aim of which is to predict downwind deposition of spray drift from aerial, ground boom and orchard/vineyard airblast pesticide applications (Hewitt, 2002).

The fundamental premise of the cooperative SDTF effort was that off-site drift is primarily a function of application techniques, environmental conditions, and the physical properties of a tank mix and that, after the formation of the spray droplets, is independent of the specific active ingredient. As such, spray drift for different tank mixes applied using the same application equipment can be presumed to be generically related to physical solution properties and not the chemistry of the active ingredient. Therefore, a comprehensive database of off-site drift and deposition phenomena could be developed independent of specific active ingredients. This generic approach is based on three general assumptions.

1. The first is that degradation and volatilization of the active ingredient during the period of spray application and deposition is negligible. Nearfield drift and deposition occur within a short time frame (30 min). Loss of the active ingredient either through degradation or volatilization must be much slower than this to assure efficacy of the compound within the field.
2. The second assumption is that the physical properties should be measured in the tank mix and tracer levels would correlate to full active-ingredient rates. It should also be noted that adjuvants were not tested completely in the SDTF studies but rather only a subset of tank mixes.
3. The third assumption is that the risk to non-target organisms can be evaluated as a two-stage process where environmental concentrations are used to estimate exposure to the contaminant and then combined with measurements of biological activity to determine risk.

*Use in South Africa*

A study by Schulz et al. (2001a) measured drift deposition of azinphos-methyl and endosulfan (applied by orchard airblast) at various distances from the point of application in the Lourens River catchment in the Western Cape. This study found that measured deposition compared very well with predicted deposition derived from SDTF regressions.

A more recent study (Nsibande et al., 2015) successfully validated the AGDISP model and highlighted its application for pesticide exposure assessment in South Africa. First, a method to sample and quantify the spray drift of atrazine applied to a sorghum crop was developed and validated. Secondly, spray application data collected during the sampling campaign (e.g. nozzle type, droplet size application rate, etc.) was used as input data to the AGDISP model to generate predicted airborne concentrations and deposition quantities of pesticide.

Spray drift monitoring was conducted during spraying of weeds in a sorghum field in Standerton, South Africa, under calm meteorological conditions. The herbicide solution contained atrazine (which was targeted as a drift tracer) and was applied using a boom sprayer. Both deposition and airborne spray drift samples were collected downwind of the application area using chromatography paper

fallout sheets and PUF high volume samplers, respectively. Additionally, data required by the AGDISP model as input for drift simulations was obtained from the farmer. Meteorological information was measured using a portable weather station and the droplet size distribution (DSD) was determined using magnesium oxide coated slides. Three different sets of droplet distributions were thus obtained. The predicted model simulations were compared to measured data to determine the accuracy of the model.

To determine the important input factors of the model that significantly affect spray drift predictions, sensitivity tests were conducted using ranges based on maximum and minimum values recorded during the sampling period. Finally, the model was used to simulate spray drift for different application scenarios for the study areas of interest. The results of the study can be summarised as follows:

- The active pesticide ingredient, namely atrazine, was successfully used to monitor downwind spray drift under local conditions during application due to its stability and compatibility with the instrumentation that was used.
- A good correlation between model predicted and field experimental results was obtained for airborne levels which suggests that the model can be used to provide a good estimate for airborne drift in risk assessment studies or for regulatory purposes.
- Compared to the experimental results, the model under-predicted deposition by up to one order of magnitude compared to the GC-NPD results and even more compared to the DSA-TOFMS results close to the field.
- Sensitivity studies showed that the model was strongly dependent on droplet size as supported by other studies. Among the meteorological parameters, wind speed was the most significant factor.
- This study validated the AGDISP model under South African conditions using the pesticide active ingredient up to 400 m from the application site.

*Ganzelmeier Drift Values*

In Europe drift loadings are calculated based on drift values derived by the German BBA (Ganzelmeier et al., 1995; Rautmann et al., 1999) which divided crops into five groups (arable crops, fruit crops (orchards), grapevines, hops and vegetables/ornamentals/small fruit) with additional distinction made between the early and late growth stages for fruit crops and grapevines and a crop height distinction for vegetables/ornamentals/small fruit. For each crop type and growth stage combination, experimental spray drift deposition data have been compiled as a function of distance from the edge of the treated field (Table 3-4). The 90$^{th}$ percentile drift values were calculated for each distance and used to generate a 90th percentile regression curve for each crop and growth stage combination. For lower tier risk assessments in Europe drift values representative of a 1 m “no spray zone” for arable crops and a 3 m “no spray zone” for vines, orchards and hops have been selected as these represent the minimum default distance taking into account the ubiquitous presence of natural

buffers. Seed and granular treatments will always have drift of 0% for all treatments and aerial drift loadings have been set to 33.2% for all applications.

Table 3-3 90th percentile drift values (% of application) based on crop type and distance from the point of application.

| Distance (meter) | Vine (early) | Vine (late) | Fruit (early) | Fruit (late) | Arable (early) | Arable (late) |
|---|---|---|---|---|---|---|
| 1 | 23.2 | 20 | 46.2 | 26.7 | 4 | 5 |
| 2 | 8 | 12 | 34.5 | 22.3 | 1.6 | 1.8 |
| 3 | 4.9 | 7.5 | 29.6 | 19.6 | 0.9 | 1.4 |
| 4 | 2.6 | 5.8 | 23.8 | 15.3 | 0.6 | 1.0 |
| 5 | 1.6 | 5.2 | 19.5 | 10.1 | 0.5 | 0.7 |
| 7.5 | 1 | 2.6 | 14.1 | 6.4 | 0.3 | 0.5 |
| 10 | 0.4 | 1.7 | 10.6 | 4.4 | 0.3 | 0.4 |
| 15 | 0.2 | 0.8 | 6.2 | 2.5 | 0.2 | 0.2 |
| 20 | 0.1 | 0.4 | 4.2 | 1.4 | 0.1 | 0.1 |
| 30 | 0.1 | 0.2 | 2.0 | 0.6 | 0.1 | 0.1 |
| 40 | 0.1 | 0.2 | 0.4 | 0.6 | 0.1 | 0.1 |
| 50 | 0.1 | 0.2 | 0.2 | 0.6 | 0.1 | 0.1 |

*Use in South Africa*

Drift values generated by the German BBA have been successfully validated in a number of studies conducted in the Lourens River catchment. Deposition of azinphos-methyl and endosulfan was accurately predicted by the Ganzelmeier drift values at varying distances from the point of application (0, 5, 10 and 15 m) (Schulz et al., 2001). In another study drift deposition of azinphos-methyl in a stream adjacent to a pear orchard was accurately predicted by the Ganzelmeier drift values (Dabrowski et al., 2005).

## 3.5. Model Sensitivity

Previous studies have performed sensitivity analysis on the PRZM model. Dubus et al. (2003a) adopted a simple approach which is referred to as one-at-a-time sensitivity analysis. This involves varying input parameters independently, one at a time, all other parameters being constant and observing the influence on model predictions. The assessment of model sensitivity was based on the ratio of the relative variation in model output to the relative variation in model input. Dabrowski et al. (2013) performed a similar analysis on the OECD runoff model. For this analysis, runoff input parameters were varied in increments within realistic minimum and maximum ranges. In both studies physicochemical properties of the pesticides – Kd and half-life – were shown to have the most significant influence on model output results. Dubus et al. (2003a) also highlighted field capacity and bulk density of the soil as being important.

The sorption coefficient (Kd) is a measure of the extent of interaction of the chemical with soil and its components and is a salient characteristic that plays an important role in these models.

Physicochemical properties of pesticides are known to be spatially variable. Soil characteristics, such as pH, particle size distribution or texture, amount and type of clay, and amount and quality of organic carbon (OC), vary widely between agroclimatic regions. Despite soil composition heterogeneity, most theoretical descriptions of pesticide sorption have been based on the predictive models that use average Kd values. Moreover, studies to predict pesticide fate often lack direct measurements of Kd, and therefore, it is common practice to use data from the literature, usually mean values calculated from a database – this is particularly the case in South Africa. These and other values of soil properties contained in such databases are used in environmental fate models. Variability in the sorption distribution coefficient Kd can generally be reduced by normalising it to the organic carbon content, but the variability of the resulting Koc often remains considerable (for example Koc of atrazine varied from 125 to 250 within a 6.25 ha field (Ahmad and Rahman, 2009).

As discussed in the literature review, physicochemical properties of pesticides registered for use in South Africa are generally determined in laboratory or field experiments, the origin of which is unknown (i.e. it is not specifically required that environmental fate parameters are derived using relevant South African soils). Even if the experiments were conducted under relevant South African conditions the inherent spatial variability in these parameters would still result in relatively high uncertainty associated with model outputs. As such there is often a degree of reservation about using physicochemical data from more temperate climates as combinations of the chemical properties as well as site-specific conditions determine the fate and behaviour of pesticides (Daam and Van den Brink, 2010). These conditions vary greatly among different agro-ecological zones making the direct extrapolation of data between geographical regions very challenging (Ahmad and Kookana, 2007). However, Wauchope et al. (2002) found that while there is often variation in the Koc value of a specific pesticide, the values are adequate for discriminating between the relative mobility of a number of different pesticides. A study on the behaviour of three pesticides in South African soils reported similar Koc values to those reported in the international literature, while half-lives were generally longer in South African soils (Meinhardt, 2009). Meinhardt (2009) however recommended the use of fate models in pesticide registration and further recommended that a range of adsorption coefficients be used for each pesticide so as to ensure that worst-case scenarios are accounted for. Pesticides with Koc values higher than 1000 were found almost exclusively in the sediment phase (i.e. azinphos-methyl, chlorpyrifos, flusilazole, methyl parathion and prothiofos), while those below 1000 were found almost exclusively in the water phase (i.e. carbaryl and dimethomorph).

However, considering the sensitivity (and associated uncertainty) of environmental fate models to these physicochemical properties Dubus et al. (2003a) recommend that future research should concentrate on quantifying the impact these uncertainties have on exposure assessments and on developing procedures that enable their integration within probabilistic assessments.

# 4. A Bayesian Network for Pesticide Fate and Transport

*JM Dabrowski*

## 4.1. Background

In environmental management, decisions are often based on either expert judgement or on complex quantitative models that consider only a small subset of environmental processes within a complex system. One of the main criticisms of current risk assessment approaches employed in pesticide registration is their deterministic approach, specifically relying on single data points to represent otherwise highly variable environmental and physicochemical variables. As such model outputs can be regarded as highly uncertain. Worst-case scenarios are therefore often adopted to ensure a conservative, protective approach. Current off-the shelf models (i.e. PRZM) are not conducive to performing probabilistic exposure assessments as they are specifically designed to capture single data points for input variables. Any attempt at performing probabilistic assessments with these models involves running the model repeatedly, each time varying input parameters, which is very costly (in terms of time and processing power required).

The risk assessment framework is an iterative process that seeks to address limitations in environmental management by offering a formal and adaptive approach to decision-making (Hart et al., 2005). The framework aims to improve our understanding of how a system functions, and how decisions to manage a system affect ecological assets. Being an adaptive approach to environmental management, the process acknowledges that often uncertainties in our understanding of a complex system may be typically large at first, but with further data collection and analysis, these uncertainties can be reduced.

Traditionally, models used in ecological risk assessments have tended to be restricted to single hazard assessments, with poor quantification of uncertainties, and poor capacity for fitting into an iterative and adaptive management approaches (Pollino and Hart, 2005). The goal of any modelling effort is to integrate information in such a manner as to provide a coherent view that aids reasoning and facilitates the decision making process in the face of uncertainty. Based on model results, either a choice of an interpretation of reality is realised or a selection of a course of action is achieved. One tool that has shown potential in meeting the modelling needs of risk assessments is Bayesian Networks (BNs). BNs offer a pragmatic and scientifically credible approach to modelling complex ecological systems, where substantial uncertainties exist (Pollino et al., 2007).

If good quality information is available then the decision making process may proceed with a high level of confidence. Unfortunately environmental management is often complex and often involves multiple stakeholders and numerous cause-and-effect variables. This means that often decision making has to occur based on a mix of evidence and intuition. Thus one must very often rely on probabilistic tools to account for inadequate datasets or integrate information from different data

sources into a coherent logical framework. In simple terms, a BN is a model that does not rely exclusively on historical information or current trends. Instead, it represents cause and probable effects (and likelihoods) via an intuitive graphical interface thus facilitating a form of automated reasoning.

This aim of this chapter is to design a BN network that could potentially be used in risk assessment for pesticide registration in South Africa. The intention of this approach is to account for uncertainty in the risk assessment process, an aspect which is currently not considered in any risk assessment approach for pesticide registration throughout the rest of the world. Ultimately this approach will be compared to a more conventional deterministic approach using well established pesticide fate and transport models (e.g. PRZM). Both approaches will require the derivation of relevant environmental data (e.g. weather, soil characteristics, etc.) as input into the model. The BN will however be able to consider probability distributions of such data whereas the deterministic approach will utilise single data points from these distributions (generally representative of worst-case scenarios). This chapter focusses on the preliminary design of a BN with the objective being to estimate the percentage of an applied pesticide that would be lost in runoff. The model will be developed further (i.e. to include spray drift and estimate a PEC) as the project progresses.

## 4.2. Building a Conceptual Model

The ecological risk assessment framework needs to be formulated as a BN graph, providing an opportunity for stakeholders and decision-makers to produce a first-cut assessment of the important variables, decisions, outcomes and relationships in the problem. Variables in a BN are represented by nodes in the graph. The three types of BN graph nodes include:

- Decision nodes (representing sets of distinct management alternatives),
- Utility nodes (representing costs and other value measures) and
- State nodes (representing variables that can exist in any of several separate states with a certain probability).

The BN graph serves as a reference for later data analysis and information gathering used to refine the graph structure and infer probability distributions. The following sub-sections highlight relevant steps for building the BN graph (Ames et al., 2005).

### Identify Management Endpoints

Selection of endpoints at the outset helps keep the BN focused only on variables significant to the decision problem under investigation. If this is done with the direct input of stakeholders, it has the effect of bringing different interests together to agree on a set of endpoints for evaluation. For the purposes of this initial model development the percentage of an applied pesticide lost in runoff is the endpoint of interest.

#### Identify Critical Intermediate and Exogenous Variables

A minimum number of intermediate state nodes should be selected to define the relationship between management options and endpoints while capturing all variables that decision-makers and stakeholders consider important. In a group setting, this process can iterate until all parties involved agree on a single BN graph structure. Exogenous variables that drive the system, but are not managed (e.g. precipitation), are also identified at this stage.

#### Establish Discretization States for Variables

Terciles or quartiles of the data can be convenient discretization states when all that is needed is a distinction between “high”, “medium” and “low.” Alternatively, it may be more meaningful to stakeholders and decision-makers if the discretization is based on values critical to the management problem (e.g. whether PECs are higher or lower than a toxicity endpoint).

#### Identify Data Sources

It is important to identify data sources at the outset to ensure that all available and relevant information is used in the BN model. This activity may help one to refine the BN model by eliminating graph nodes where no information is available and adding nodes where information is available. This activity will also help identify data gaps where expert judgment may be needed to characterize the relationship between variables.

#### Plan for Use of Probabilistic Results

For some environmental problems, results may be required or expected to be “true” or “false” (e.g. “the risk of the pesticide levels in runoff to the aquatic ecosystem is unacceptable”). However, by definition, results from a BN analysis are probabilistic (e.g. “there is a high probability that pesticide inn runoff will result in an unacceptable risk to the aquatic ecosystem”). Because of this, it is important to establish early on how probabilistic results will be used to address the problem. For example, the plan may be to convert probabilistic results into binary results using some threshold (e.g. if the probability of unacceptable risk to the aquatic ecosystem is over 70% then the risk is unacceptable). It is also useful to report results in terms of risk (e.g. “under proposed label use, there is a 20% chance that pesticide concentrations derived from runoff will exceed a certain risk threshold”).

### 4.3. Bayesian Net Model Development

The BN is designed to represent a representative catchment area identified as a potential worst-case runoff area. The intention of the approach is to develop probability distributions of the various climatic (e.g. precipitation) and geographical (i.e. precipitation, soil type, slope, hydrology) features of the catchment that influence pesticide runoff, such that the output of the model is a probability of a certain

percentage pesticide loss in runoff for any given agricultural field in the catchment (i.e. given the specific climatic and geographic conditions for this catchment we can expect such a probability that pesticides will exceed a certain level). This addresses the uncertainty associated with choosing a single value to represent each of these variables (as normally undertaken in a deterministic approach). In addition using a BN approach allows for uncertainty to be considered for the physicochemical parameters that are used in exposure assessments. These parameters are the Koc and half-life of the pesticide. It is well known that these parameters are variable, with the result being that selecting a single value to represent these parameters may lead to over or under estimation of the mobility of a pesticide and the associated risk in the environment. The purpose of the BN is for registering a pesticide and will therefore not provide any kind of spatial indication of where contamination is likely to occur, but rather the percentage of an applied pesticide that is likely to be lost in runoff and (as the model is developed further) the probability of different PECs occurring and the probability of risk associated with these PECs.

The first step in preparing a BN is to develop a conceptual diagram to portray the associations among relevant factors that influence the movement of pesticides from the area of application into nearby water resources. Nodes (displayed as boxes) represent variables, and arcs (displayed as arrows) are used to indicate a relationship between the nodes. This section describes a conceptual diagram to predict the risk of pesticide application in a catchment. At this stage of development the diagram is not representative of a specific catchment (i.e. a catchment representative of a specific agricultural production in South Africa) but rather provides a generic template as to the factors that influence pesticide transport in a catchment and how these should be represented in a BN. Components of the diagram are constructed with the expectation that values or quantifiable estimates and relationships can be found to generate a useful BN that could be applied to a number of catchments (or exposure scenarios) representative of typical agricultural production in South Africa. Therefore, a key aspect of generating the conceptual diagram, besides the obvious causal connections that are identified, is whether data are available to populate a node or relationship of the diagram. If not, the data will have to be collected or a different structure with different data will have to be used.

**Problem Formulation**

Pesticides, due to their mode of action, pose potentially serious risks to biota in aquatic ecosystems (algae, plants, invertebrates and fish). For this reason a risk assessment is required at the point of registration in order to determine whether the pesticide poses acceptable risks to the environment under the prescribed conditions of use. This involves comparing estimates of environmental exposure (i.e. PECs) to effects data (i.e. toxicity endpoints). A number of factors influence the transport of pesticides into water bodies. PECs are therefore dependant on these factors as well as the hydrological characteristics of the water body into which the pesticides are transported.

**Conceptual Diagram for Evaluating Pesticide Risk to the Aquatic Ecosystem**

The conceptual diagram should include the major factors contributing to the transport of pesticides from the point of application into a nearby water body and the PECs that will result from this transport. For surface waters runoff and spray drift therefore need to be considered. At this stage of development only runoff is considered. Management actions that influence these factors could also be considered and included in a BN for higher tier risk assessments (i.e. if risk is considered unacceptable in lower tier assessments, the influence of management actions may be considered in a higher tier assessment). Management actions that reduce the transport of pesticides can be evaluated by changes in the risk that could be expected to occur.

The approach adopted in the development of the conceptual model was to adopt a simple modelling approach that accounts for the most important factors that influence pesticide transport. The advantage of this approach is that while the processes that influence transport are simplified it is possible to generate probability distributions for most of them (from measured or modelled data or expert elicitation). In this way variability in these input parameters and associated uncertainty in exposure estimates is considered in the risk assessment. The OECD runoff model (OECD, 1998) was used as the basis upon which to develop the conceptual model and the nodes represent important relationships described in this equation (see section 3.2).

While more complex relationships accounting for more detailed processes could be incorporated into the BN (e.g. evapotranspiration and foliar decay and wash-off are considered in the PRZM model) the large number of relationships between nodes that need to be captured in the BN and the effort in deriving probability distributions for many of these relationships through observed or modelled data or expert elicitation would render the network too cumbersome for use.

*Runoff Transport Sub-Models*

The OECD runoff equation was used to develop a conceptual model of the factors that influence the movement of pesticides in runoff. In essence there are three sub-models that make up the runoff transport component of the BN. These are:

1. The runoff model, which estimates the quantity of runoff the leaves an agricultural field following a rainfall event. This is determined by a number of factors including:
    a. The amount of rainfall (precipitation)
    b. The hydrological soil properties (which in combination with the crop type is used to determine the SCS curve number used for calculating runoff)
    c. The slope of the field
2. The first order kinetic model, which estimates the proportion of applied pesticide available for runoff following application. This is determined by the following factors:
    a. The Koc of the pesticides
    b. The % organic carbon of the soil

c. The half-life of the pesticides
d. The number of days passed between application of the pesticide and the occurrence of the rainfall event

3. The application model, which determines the quantity of pesticide applied. This is determined by the following factors:
    a. The application rate
    b. The area (hectares)

The outputs of these sub-models are combined to quantify the amount of pesticide leaving the field in runoff, which can then be used to calculate the PEC as part of the exposure assessment.

*Endpoints*

The goal of the registration of pesticides using a Bayesian approach is to determine whether pesticides (used as directed) pose an unacceptable risk to aquatic ecosystem health. The endpoint for the BN developed thus far is the quantity of an applied pesticide that leaves the field after runoff (as a percentage of the applied pesticide).

## 4.4. Model Inference

**Critical Intermediate and Exogenous Variables**

Exogenous variables include precipitation, hydrological soil group, slope and % organic carbon. These are all variables that directly influence runoff of pesticides but are not managed (or controlled). Precipitation, hydrological soil group and slope are the primary drivers for determining the quantity of runoff water that leaves an agricultural field and enters the water resource. Organic carbon % is the primary driver for influencing the extent to which pesticides bind to organic carbon. The other driver is the Kd of the pesticide itself, however this is determined by the physicochemical properties and is therefore a pre-determined state (and not an exogenous variable).

**Runoff**

The quantity of runoff leaving a field following a rainfall event is required to estimate pesticide loading associated with turnoff. According to the OECD equation, runoff is primarily dependent on the quantity of rainfall and the type of soil on which a crop is grown. The original equation utilises a model derived by Lutz and Maniak (1992) to estimate runoff volume based on the amount of rainfall (mm), soil type (sandy or loamy), soil moisture (high or low) and surface cover (bare or covered). For this BN, runoff volume was determined using the more widely used SCS runoff curve number method.

The crop type and hydrological soil group determine the SCS runoff curve number (CN). The CN has a range from 30 to 100; lower numbers indicate low runoff potential while larger numbers are for increasing runoff potential. The lower the curve number, the more permeable the soil is. The amount

of precipitation, together with the runoff curve number determines the quantity of runoff expected to occur (Figure 4-1).

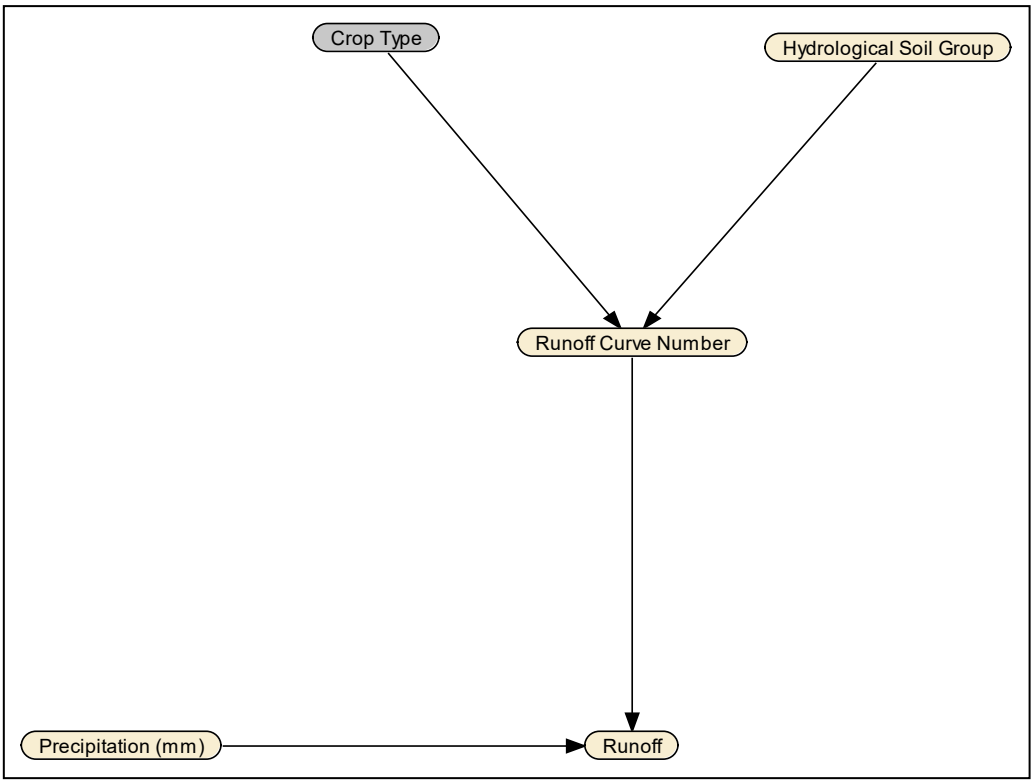


Figure 4-1 Conceptual runoff sub-model

**Pesticide Fate**

This sub-model describes the fate of the pesticide in the agricultural field after application and provides an estimate of the amount of pesticide that is available for loss via runoff. The amount of pesticide available for runoff is dependant the following factors:

a) the degradation of the pesticide (i.e. the proportion of pesticide that has degraded since the last application)
b) the proportion of pesticide that remains sorbed to organic carbon in the soil.

The proportion of pesticide available after degradation is dependent on two factors:

- The half-life of the pesticide in soil (i.e. the number of days taken for half of the quantity of pesticide to degrade into metabolites).
- The number of days that have passed since the last application.

Of the amount of pesticide available after degradation, only a fraction of this will be available for runoff. Adsorption of chemicals on soils or sediments is a major factor in the transportation of pesticides. This is dependent on the Kd (adsorption-desorption distribution coefficient) of the pesticide

which is a function of the Koc (organic carbon-water partition coefficient) of the pesticide and the organic carbon content of the soil (Figure 4-2).

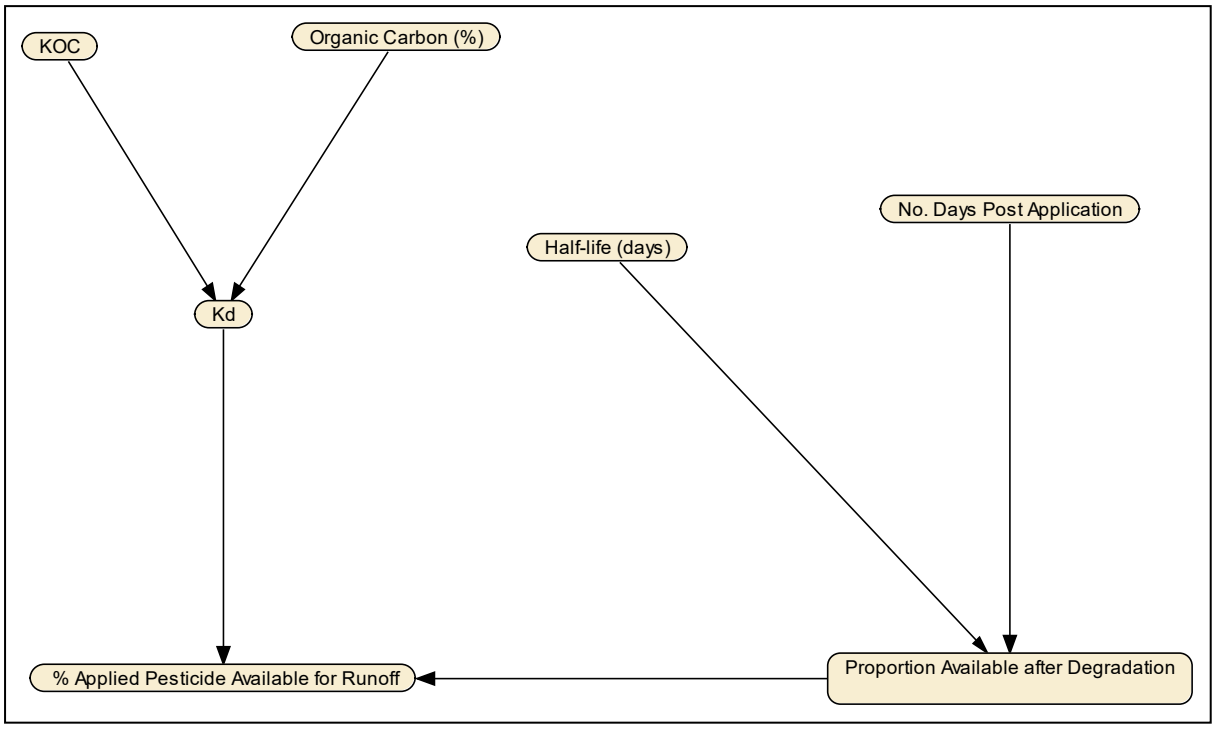


Figure 4-2 Conceptual pesticide fate model.

**Correction Factor**

According to the OECD model, the amount of pesticide lost in runoff is dependent on the slope of the agricultural field (steeper slopes will facilitate the rapid transport of dissolved pesticides while flat fields will show lower rates of runoff) and the foliar interception (i.e. the proportion of pesticide that lands on the soil surface after interception by plant foliage) (Figure 4-3).

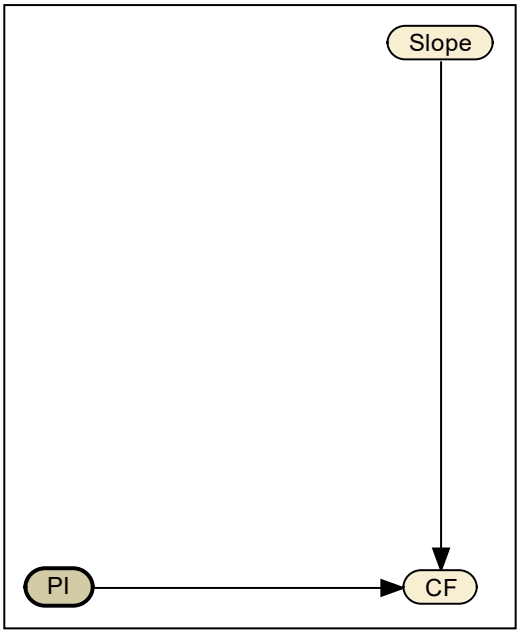


Figure 4-3 Conceptual correction factor sub-model.

**Full BN**

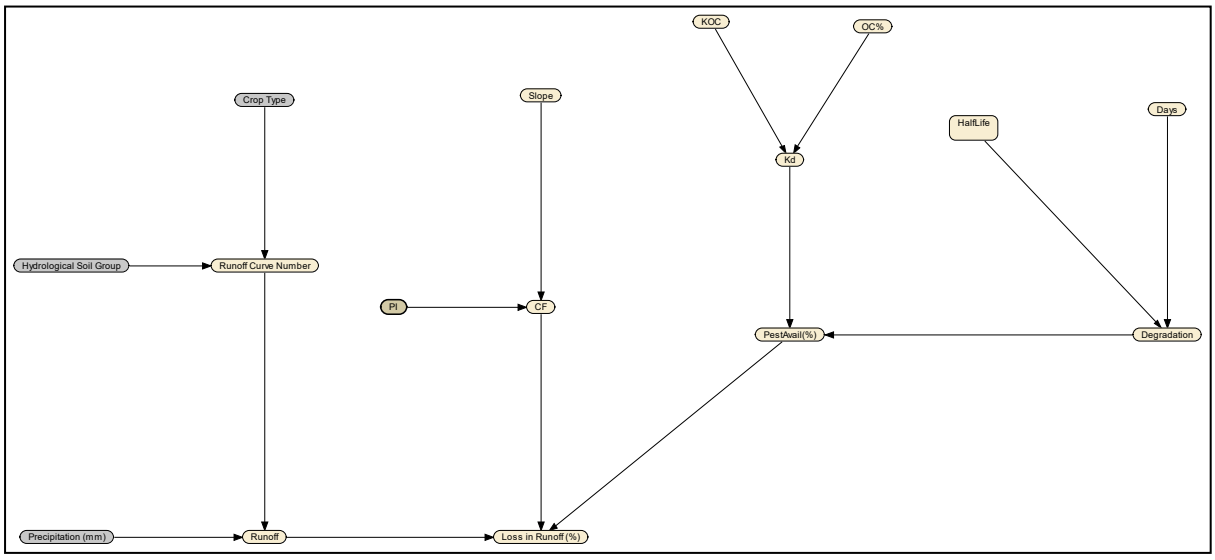


Figure 4-4 Conceptual model showing how the runoff, pesticide fate and correction factor sub-models influence the loss of pesticide in runoff (as a percentage of the applied pesticide).

## 4.5. Data Sources and Data Acquisition

### Runoff

*Hydrological Soil Group*

ACRU is a agrohydrological multi-purpose model which integrates the various water budgeting and runoff producing components of the terrestrial hydrological system with risk analysis, and can be applied in design hydrology, crop yield modelling, reservoir yield simulation, irrigation water demand/supply, water resources assessment, planning optimum water resource utilisation and resolving conflicting demands on water resources.

ACRU simulates runoff volumes from the land surface using the SCS curve method developed by the USDA. As part of the development of the ACRU model specific curve numbers were developed for different combinations of land use and soil type in South Africa (Table 4-1). Land use categories include those of typical crop types produced in South Africa and include row crops, sugar cane, small grain crops and orchards. The ACRU manual provides a table of hydrological categories for each soil form and series (i.e. binomial classification; Table 4-2). These categories are A, A/B, B, B/C, C, C/D and D which correspond to low runoff potential (A) up to high runoff potential (D).

Table 4-1 Runoff curve numbers for different combinations of land use and hydrological soil group (Smithers and Schulze, 1995).

| Land Cover Class | Land Treatment/ Practice/Description | Stormflow Potential | Hydrological Soil Group | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | A | A/B | B | B/C | C | C/D | D |
| Fallow | 1 = Straight row | | 77 | 82 | 86 | 89 | 91 | 93 | 94 |
| | 2 = Straight row + conservation tillage | High | 75 | 80 | 84 | 87 | 89 | 91 | 92 |
| | 3 = Straight row + conservation tillage | Low | 74 | 79 | 83 | 85 | 87 | 89 | 90 |
| Row Crops | 1 = Straight row | High | 72 | 77 | 81 | 85 | 88 | 90 | 91 |
| | 2 = Straight row | Low | 67 | 73 | 78 | 82 | 85 | 87 | 89 |
| | 3 = Straight row + conservation tillage | High | 71 | 75 | 79 | 83 | 86 | 88 | 89 |
| | 4 = Straight row + conservation tillage | Low | 64 | 70 | 75 | 79 | 82 | 84 | 85 |
| | 5 = Planted on contour | High | 70 | 75 | 79 | 82 | 84 | 86 | 88 |
| | 6 = Planted on contour | Low | 65 | 69 | 75 | 79 | 82 | 84 | 86 |
| | 7 = Planted on contour + conservation tillage | High | 69 | 74 | 78 | 81 | 83 | 85 | 87 |
| | 8 = Planted on contour + conservation tillage | Low | 64 | 70 | 74 | 78 | 80 | 82 | 84 |
| | 9 = Conservation structures | High | 66 | 70 | 74 | 77 | 80 | 82 | 82 |
| | 10 = Conservation structures | Low | 62 | 67 | 71 | 75 | 78 | 80 | 81 |
| | 11 = Conservation structures + conservation tillage | High | 65 | 70 | 73 | 76 | 79 | 80 | 81 |
| | | Low | 61 | 66 | 70 | 73 | 76 | 78 | 79 |
| | 12 = Conservation structures + conservation tillage | | | | | | | | |
| Garden Crops | 1 = Straight row | High | 68 | 71 | 75 | 79 | 81 | 83 | 84 |
| | 2 = Straight row | Low | 45 | 56 | 66 | 72 | 77 | 80 | 83 |
| Small Grain | 1 = Straight row | High | 65 | 71 | 76 | 80 | 84 | 86 | 88 |
| | 2 = Straight row | Low | 63 | 69 | 75 | 79 | 83 | 85 | 87 |
| | 3 = Straight row + conservation tillage | High | 64 | 70 | 74 | 78 | 82 | 84 | 86 |
| | 4 = Straight row + conservation tillage | Low | 60 | 67 | 72 | 76 | 80 | 82 | 84 |
| | 5 = Planted on contour | High | 63 | 69 | 74 | 79 | 82 | 84 | 85 |
| | 6 = Planted on contour | Low | 61 | 67 | 73 | 78 | 81 | 83 | 84 |
| | 7 = Planted on contour + conservation tillage | High | 62 | 68 | 73 | 77 | 81 | 83 | 84 |
| | 8 = Planted on contour + conservation tillage | Low | 60 | 66 | 72 | 76 | 79 | 81 | 82 |
| | 9 = Planted on contour - winter rainfall region | Low | 63 | 66 | 70 | 75 | 78 | 80 | 81 |
| | 10 = Conservation structures | High | 61 | 67 | 72 | 76 | 79 | 81 | 82 |
| | 11 = Conservation structures | Low | 59 | 65 | 70 | 75 | 78 | 80 | 81 |
| | 12 = Conservation structures + conservation tillage | High | 60 | 67 | 71 | 75 | 78 | 80 | 81 |
| | | Low | 58 | 64 | 69 | 73 | 76 | 78 | 79 |
| | 13 = Conservation structures + conservation tillage | | | | | | | | |
| Close Seeded Legumes or Rotational Meadow | 1 = Straight Row | High | 66 | 72 | 77 | 81 | 85 | 87 | 89 |
| | 2 = Straight Row | Low | 58 | 65 | 72 | 75 | 81 | 84 | 85 |
| | 3 = Planted on contour | High | 64 | 70 | 75 | 80 | 83 | 84 | 85 |
| | 4 = Planted on contour | Low | 55 | 63 | 69 | 74 | 78 | 81 | 83 |
| | 5 = Conservation structures | High | 63 | 68 | 73 | 77 | 80 | 82 | 83 |
| | 6 = Conservation structures | Low | 51 | 60 | 67 | 72 | 76 | 78 | 80 |
| Sugarcane | 1 = Straight row: trash burnt | | 43 | 55 | 65 | 72 | 77 | 80 | 82 |
| | 2 = Straight row: trash mulch | | 45 | 56 | 66 | 72 | 77 | 80 | 83 |
| | 3 = Straight row: limited cover | | 67 | 73 | 78 | 82 | 85 | 87 | 89 |
| | 4 = Straight row: partial cover | | 49 | 60 | 69 | 73 | 79 | 82 | 84 |
| | 5 = Straight row: complete cover | | 39 | 50 | 61 | 68 | 74 | 78 | 80 |
| | 6 = Conservation structures: limited cover | | 65 | 70 | 75 | 79 | 82 | 84 | 86 |
| | 7 = Conservation structures: partial cover | | 25 | 46 | 59 | 67 | 75 | 80 | 83 |
| | 8 = Conservation structures: complete cover | | 6 | 14 | 35 | 59 | 70 | 75 | 79 |

Table 4-2 Example of hydrological soil group (or SCS Grouping) for different soil forms and series in South Africa (Smithers and Schulze, 1995).

| Soil Form | Code | Soil Series | SCS Grouping | SCS Adjustment Factor | Clay Distribution Model | Typical Texture Class | Interflow Potential | Erosion Hazard Rating |
|---|---|---|---|---|---|---|---|---|
| ARCADIA | Ar 10 | Mngazi | C/D | | 2e | Cl | 0 | Low |
| C/D | Ar 11 | Bloukrans | C/D | | 2e | Cl | 0 | High |
| | Ar 12 | Noukloof | C/D | | 2e | Cl | 0 | Low |
| | Ar 20 | Gelykvlakte | C/D | | 2e | Cl | 0 | Mod |
| | Ar 21 | Clerkness | C/D | | 2e | Cl | 0 | High |
| | Ar 22 | Zwaarkrygen | C/D | | 2e | Cl | 0 | Mod |
| | Ar 30 | Rydalvale | C/D | | 2e | Cl | 0 | Low |
| | Ar 31 | Rooidraai | C/D | | 2e | Cl | 0 | Low |
| | Ar 32 | Nagana | C/D | | 2e | Cl | 0 | Low |
| | Ar 40 | Arcadia | C/D | | 2e | Cl | 0 | Mod |
| | Ar 41 | Eenzaam | C/D | | 2e | Cl | 0 | Mod |
| | Ar 42 | Wanstead | C/D | | 2e | Cl | 0 | Mod |
| | Av 10 | Mastaba | A | +l/+t | 1a | LmSa | X | High |
| | Av 11 | Welverdiend | A | +l/+t | 1a | LmSa | X | High |
| | Av 12 | Banchory | A | +l/+t | 1a | Sa | X | High |

The WR90 soil coverage displays the spatial distribution of different soil according to the binomial classification and can therefore be used to identify probability distributions of different hydrological soil categories (i.e. A, B, C and D) within a selected catchment. These can be defined for areas where agricultural land cover occurs in the catchment (i.e. using national land cover coverages). Depending on the crop type for which a pesticide is being registered for, curve numbers can be identified using the tables in the ACRU manual.

*Precipitation*

Data on rainfall can be obtained from a number of sources previously described in Chapter 1.

**Pesticide Fate**

The pesticide fata sub-model requires physico-chemical data for the pesticide, namely the half-life and Koc. These parameters are typically supplied by the applicant seeking registration of the pesticide. As highlighted previously there is a high level of uncertainty associated with the use of these parameters in exposure assessments, particularly in the South African context. The advantage of the BN approach is that this uncertainty can be incorporated into the exposure assessment by entering alternative states for physicochemical values based on a probability distribution of measured or modelled data or on expert opinion. GIS coverages produced by the ARC and can be used to determine the probability distributions of organic carbon in the soil under agricultural land cover in the selected catchment.

### Pesticide Application

Pesticide application data (i.e. dose and rate of application) is supplied by the applicant seeking registration of the pesticide and the method of application will be dependent on the crop to which the pesticide is to be applied and the formulation of the product.

### Correction Factor

*Plant interception*

The OECD runoff equation models runoff of pesticides from the soil surface only (i.e. not from the plant surface as well). The proportion of pesticide that reaches the soil surface is heavily dependent on the foliar coverage of the crop which varies according to crop type and growth stage of the crop. For example a crop will intercept far less pesticide during the early growth stage of the plant (when the surface area of the leaf is small) compared to a later growth stage (when the surface area of the leaf is larger). Linders et al. (2007) published growth-phase specific interception factors for a number of crops for the purposes of performing exposure assessments in risk assessment. The factors are based on measured data for a number of crops grown throughout Europe and North America. Single values are provided for each crop and growth phase and can be viewed in the Appendix.

*Slope*

Probability distributions of different slope categories can be derived from a Digital Elevation Model (DEM) using GIS software. These can be derived for areas of the selected catchment under agricultural land cover.

*Buffer Zones*

The model makes provision for modifying pesticide input via runoff by including a buffer zone. Vegetated buffer zones are a recognised mitigation measure, which potentially reduce pesticide input through decreasing the rate of flow and runoff, promoting infiltration, settling of sediment and adsorption of pesticides to plant surfaces. A study performed in the Lourens River catchment (Stehle et al., 2016) showed that erosion rills located within buffer strips provide a preferential flow path, and that the efficiency of buffer strips can be significantly over-estimated if not taken into account. At lower tier assessments it is therefore recommended that the effect of buffer strips on pesticide transport be ignored. Buffer strips could however be considered in higher tier assessments, when more site specific information on the physical characteristics of the buffer strip would be required.

## 4.6. BN Model for Pesticide Registration

BNs are directed acyclic graphs structured to represent conditional independence among variables. Nodes (typically displayed as circles or boxes) in a BN represent variables, and arcs (displayed as arrows) are used to indicate a conditional relationship between the parent/s (originator/s) and child (receiver) nodes. Nodes without parents are considered 'root' nodes. The uncertainty of a root node is described by the distribution of its values, or prior probability distribution. The strength of the relationship between parent and child node is based on probabilistic evidence stored in the conditional probability table (CPT) of the child node. The CPT reflects the conditional probability of every combination of parent and child value (state), and can be constructed from:

1. Frequencies built from standard statistical methods for developing probabilities and entered directly,
2. Observations such as counts or
3. Equations, either deterministic or probabilistic.

Netica (Norsys, 2000) was the software used for this study and all BN diagrams are Netica output.

**Runoff Sub-Model**

Crop, hydrological soil group and precipitation are root nodes for this sub-model. CropType refers to the crop for which the pesticide is being registered. Because the crop type is known, there is no uncertainty (100% probability that the crop belongs to one of the four CropType categories) and the crop type can be selected (at 100% probability) in the Netica node (e.g. if the crop for which the pesticide is being registered is for apples then the state for CropType is Orchard, with 100% probability). The CropType together with the hydrological soil group (SoilType) define the distribution of runoff curve numbers that have been developed for these different combinations. The probability state of each SoilType would be determined based on the relative distribution of the different hydrological soil groups in areas of the selected catchment under agricultural land cover. For this example it is assumed that each of the hydrological soil groupings are evenly distributed across agricultural land in the selected catchment (i.e. 25% probability of occurrence for A, B, C and D, respectively). The ACRU manual (Smithers and Schulze, 1995) was used to derive a CPT for expected runoff curve numbers based on the combination of SoilType and CropType (Table 4-3; Figure 4-5).The probability associated with each combination reflects potential land management practices that may influence the rate of runoff (Table 4-3, Smithers, 1995 #1211).

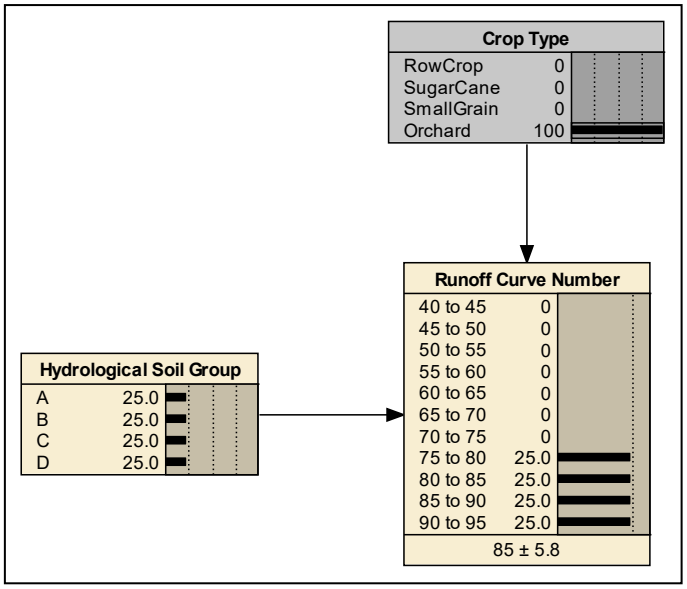


Figure 4-5 BN depicting the influence of crop type (CropType) and soil type (SoilType) on the runoff curve number (RCN)

Table 4-3 Conditional probability table for runoff curve numbers associated with different combinations of crop and soil types.

| Soil | Crop Type | 40-45 | 45-50 | 50-55 | 55-60 | 60-65 | 65-70 | 70-75 | 75-80 | 80-85 | 85-90 | 90-95 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | RowCrop | 0 | 0 | 0 | 0 | 50 | 50 | 0 | 0 | 0 | 0 | 0 |
| A | SugarCane | 20 | 40 | 0 | 0 | 0 | 40 | 0 | 0 | 0 | 0 | 0 |
| A | SmallGrain | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| A | Orchard | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 |
| B | RowCrop | 0 | 0 | 0 | 0 | 0 | 0 | 50 | 50 | 0 | 0 | 0 |
| B | SugarCane | 0 | 0 | 0 | 0 | 0 | 60 | 0 | 40 | 0 | 0 | 0 |
| B | SmallGrain | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| B | Orchard | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| C | RowCrop | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 45 | 45 | 10 | 0 |
| C | SugarCane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 80 | 20 | 0 | 0 |
| C | SmallGrain | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 50 | 50 | 0 | 0 |
| C | Orchard | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 |
| D | RowCrop | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 40 | 60 | 0 |
| D | SugarCane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 80 | 20 | 0 |
| D | SmallGrain | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 70 | 30 | 0 |
| D | Orchard | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |

The runoff curve number, together with the amount of precipitation, determine the quantity of runoff, (expressed as a ratio of the precipitation amount):

*Runoff = (P - (0.2 * (254 * ((100/RCN)-1))))^2/(P + (0.8 * (254 * ((100/RCN)-1))))*

In Netica, the “equation to table” function transfers values from the deterministic equation to the CPT using a series of random values. The number of random values that are used to generate probabilities can be set within the program and, because of the high uncertainty, 100,000 were used for all steps in this study.

Data on precipitation was retrieved from a data record for a random catchment included in the SAPWAT database. In this example the rainfall data was statistically analysed and found to have a normal distribution. For a normal distribution, an average and standard deviation are entered into the Netica software. The average daily rainfall for the selected catchment was 2.293 mm with a standard deviation 6.2615 mm and the data were entered into Netica as:

*p (Precipitation |) = NormalDist (Precipitation, 2.293, 6.2615)*

The “equation to table” function transferred values from the probabilistic equation to the CPT using a series of random values. Compiling the network (starting the model in the Netica software) provides a graphic representation of rainfall distribution on the belief bars. The distribution for rainfall was discretized into 5 mm categories (Figure 4-6). The finalised runoff BN sub-model is shown in Figure 4-7).

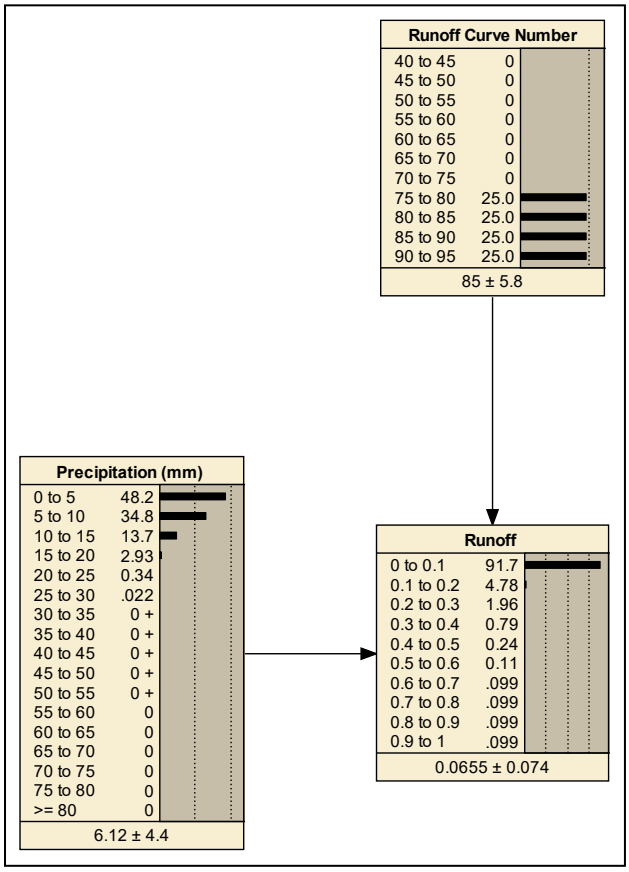


Figure 4-6 BN depicting the influence of runoff curve number (RCN) and precipitation (Precipitation) on the proportion of runoff generated relative to precipitation (Runoff).

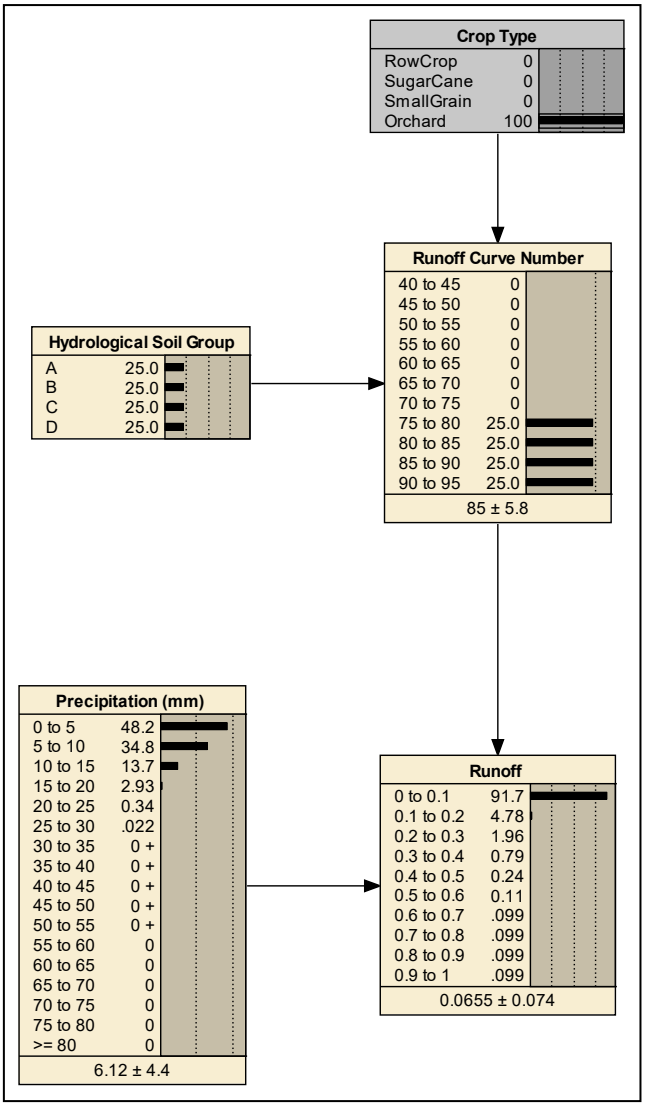


Figure 4-7 Combined runoff sub-model showing how all factors influence runoff.

### Pesticide Fate Sub-Model

Degradation of pesticide is dependent on the half-life of the pesticide and the number of days passed between application and the start of the runoff event. In the example presented here the half-life of the pesticide is 10 days. In order to account for uncertainties associated with the derivation of this half-life value, the root node HalfLife assumed an equal probability of a range of half-life values 25% higher and lower than the value of 10. In other words there is a 50% probability that the half-life value falls within the range of 7.5 to 10 days and a 50% probability that the half-life value falls within the range of 10 to 12.5 days. The number of days since application (Days) ranged from 0 to 20 in increments of 1 day, with an equal probability associated with each state. The proportion of pesticide available after degradation was calculated as follows:

$$Degradation = e^{\left(-t \times \frac{ln2}{DT_{50}}\right)}$$

where: t = time (days) since last application and the start of the runoff event and DT50 = half-life of pesticide (days). The “equation to table” function was used to transfer values from the equation to the CPT for the Degradation node using a series of random values. The output of the BN is the proportion of pesticide available for runoff and ranges from (0 to 1) (Figure 4-8).

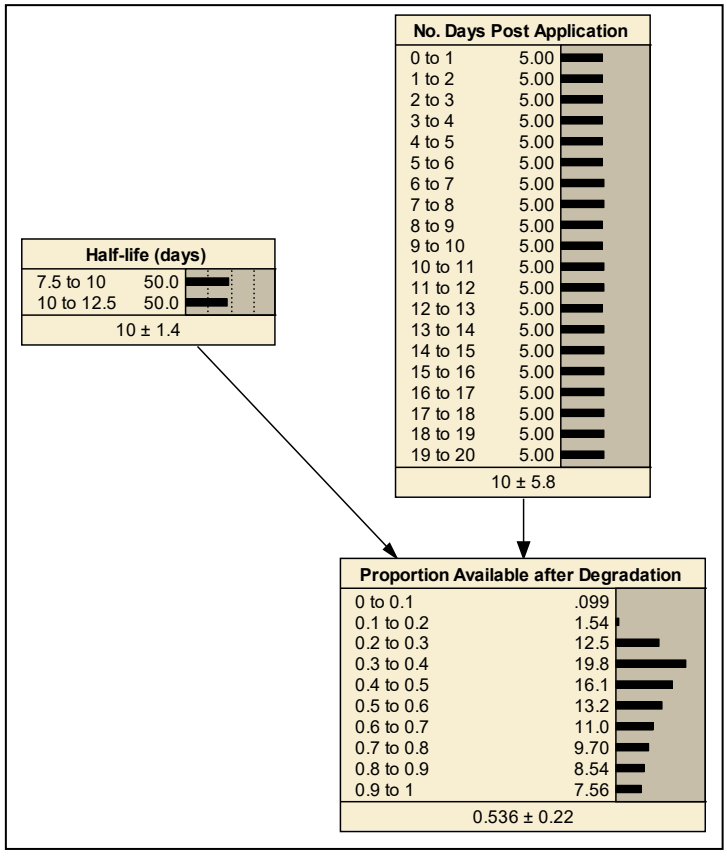


Figure 4-8 BN depicting the influence of number of days since application (Days) and half-life (HalfLife) on the proportion of pesticide degraded since application (Degraded).

The percentage (ranging from 0 to 100%) of applied pesticide unbound to organic carbon (and therefore available for runoff) is dependent on the Koc of the pesticide (1000 for this example) and organic carbon (%) in the soil. In the example presented here the organic carbon in soil (OC%) was assumed to be equally distributed between the discretised categories (0.25-0.5; 0.5-0.75; 0.75-1). Similar to the approach adopted in the degradation estimate, the root node Koc assumed an equal probability of a range of values 25% higher and lower than the value of 1000. The Kd was calculated as follows:

$$Kd = \frac{100}{1 + \left(Koc \times \frac{\%OC}{100}\right)}$$

The “equation to table” function was used to transfer values from the equation to the CPT of the Kd node using a series of random values. The output of the equation is probability of different Kd values from 0 to 100, discretized into intervals of 10 (Figure 4-9).

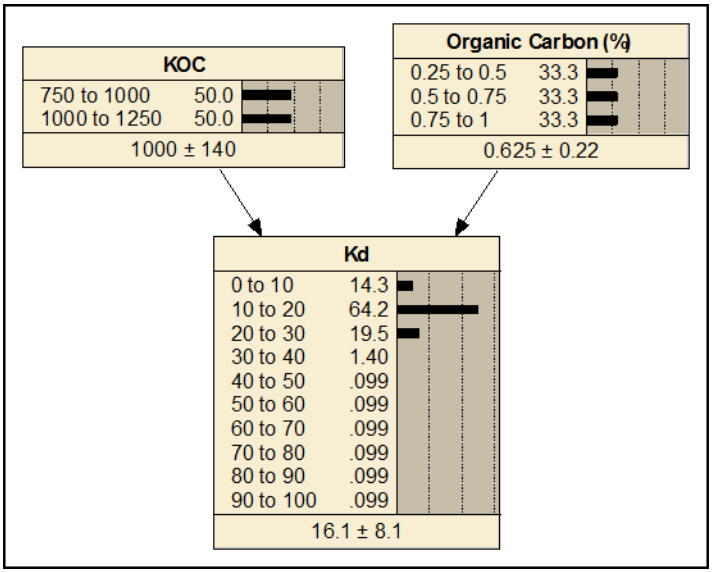


Figure 4-9 BN depicting the influence of Koc (Koc) and percentage organic carbon in soil (OC%) on the adsorption coefficient of the pesticide (Kd).

The percentage of pesticide available (PestAvail%) for runoff is dependent on the Kd and the amount available after degradation:

$$AvailablePesticide(\%) = Degradation \times Kd$$

The “equation to table” function was used to transfer values from the equation to the CPT of the PestAvail% node using a series of random values. The output of the equation is the probability that a certain proportion of the applied pesticide will be available for runoff, with states ranging from 0% (none of the applied pesticide is available for runoff) to 100% (all of the applied pesticide is available for runoff) (Figure 4-10). The full BN sub-model is shown in Figure 4-11.

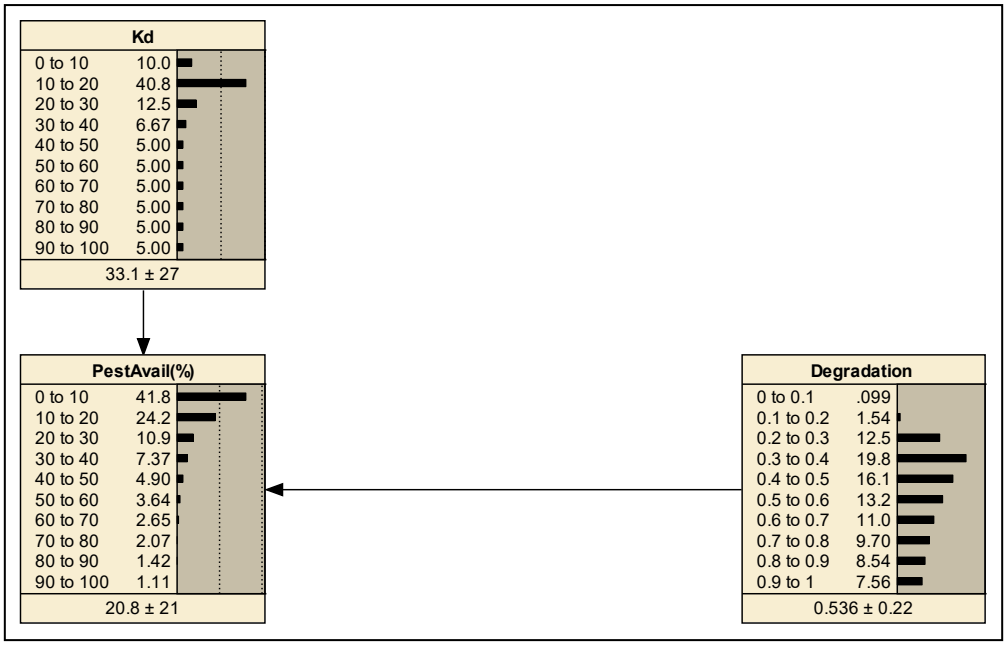


Figure 4-10 BN depicting the influence of the proportion of pesticide that has degraded (Degradation) and the adsorption coefficient of the pesticide (Kd) on the percentage of an applied pesticide available for runoff (PestAvail%).

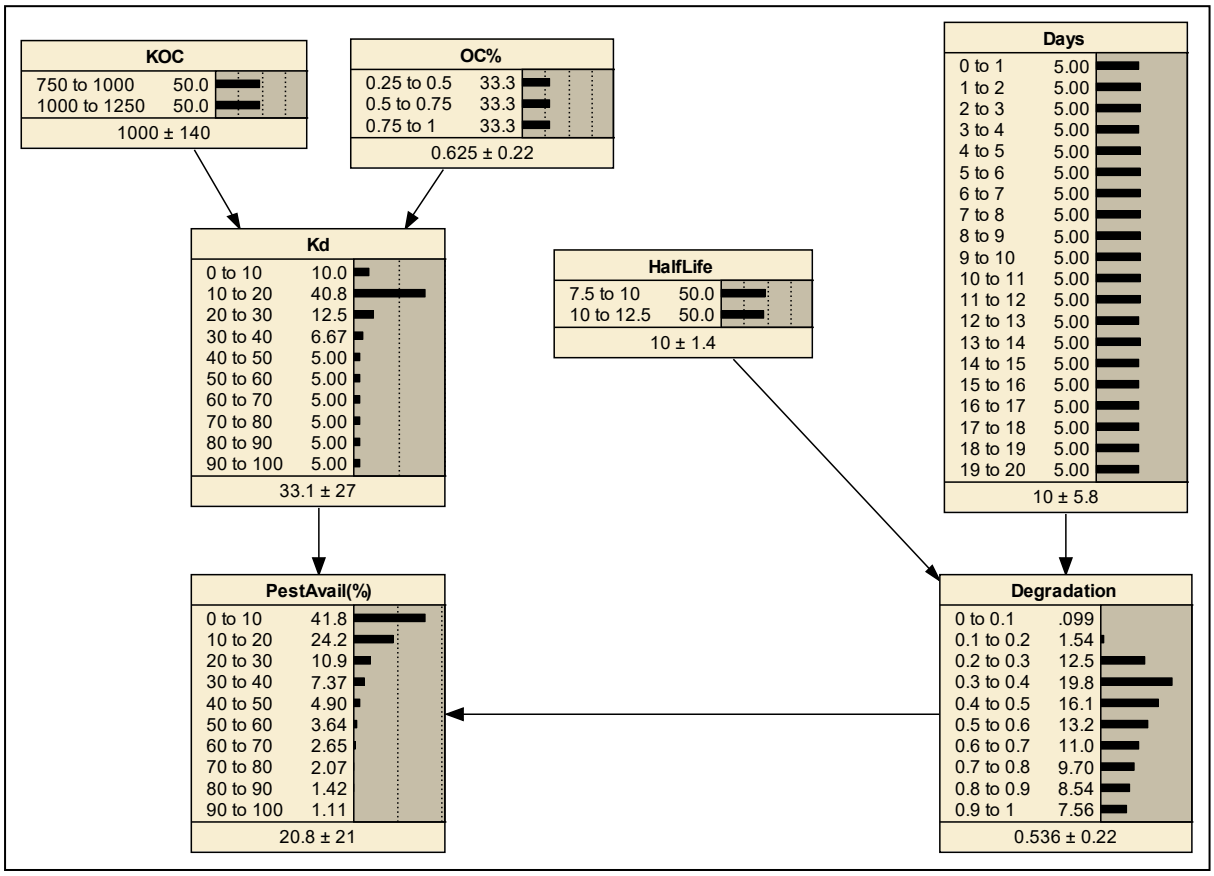


Figure 4-11 Combined pesticide availability sub-model showing how all factors influence runoff.

### Correction Factor Sub-Model

The correction factor sub-model takes the influence of slope and plant interception on total pesticide loss into account. For the example presented here, the distribution of different slope percentage classes in a selected catchment were determined using GIS. This distribution was entered as probabilities for agricultural land occurring on different slope categories in the *Slope* node. The proportion of pesticide expected to be intercepted by the crop was randomly chosen as 50%. According to the OECD equation (OECD, 1998) the correction factor (*CF*) was estimated according to the following equation:

$$CF = Slope \times PI$$

The "equation to table" function was used to transfer values from the equation to the CPTof the *CF* node using a series of random values. The output of the equation assigns probabilities to the proportion of available pesticide that will be transported in runoff, ranging from values of 0 (zero pesticide loss) to 1 (100% of the available pesticide will be transported in runoff) (Figure 4-12).

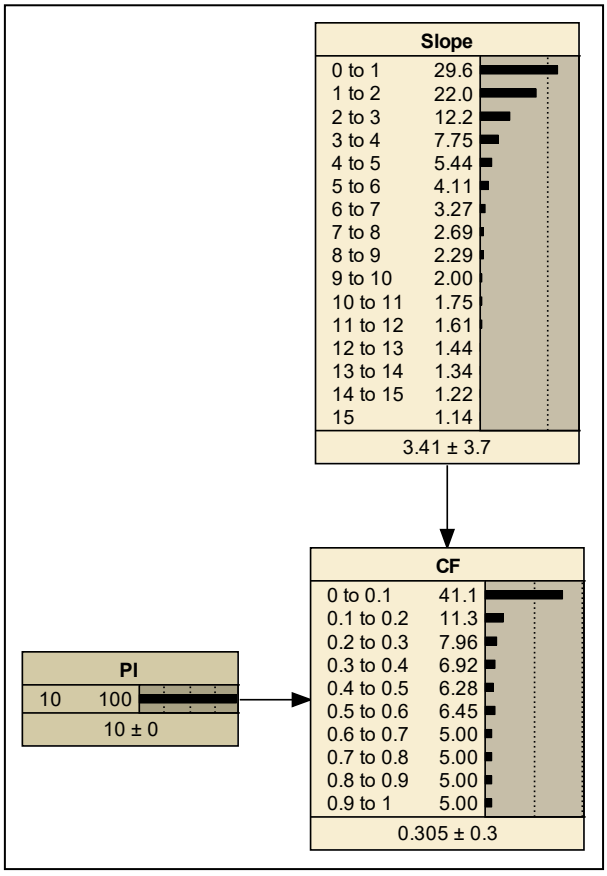


Figure 4-12 BN depicting the influence of the interception of applied pesticide by the crop (PI) and slope (Slope) on the proportion of available pesticide that will be transported in runoff (CF).

### Pesticide Loss in Runoff

The percentage of applied pesticide lost in runoff (*PestLoss%*) is determined according to the following equation:

$$PestLoss\% = Runoff \times CF \times PestAvail\%$$

The "equation to table" function was used to transfer values from the equation to the CPTof the *CF* node using a series of random values. The output of the equation assigns probabilities to the percentage categories (discretised every 0.5%) of applied pesticide that will be transported in runoff, with values ranging 0% to 100%. The full BN depicting the influence of all sub-models on determining *PestLoss%* is shown in Figure 4-13

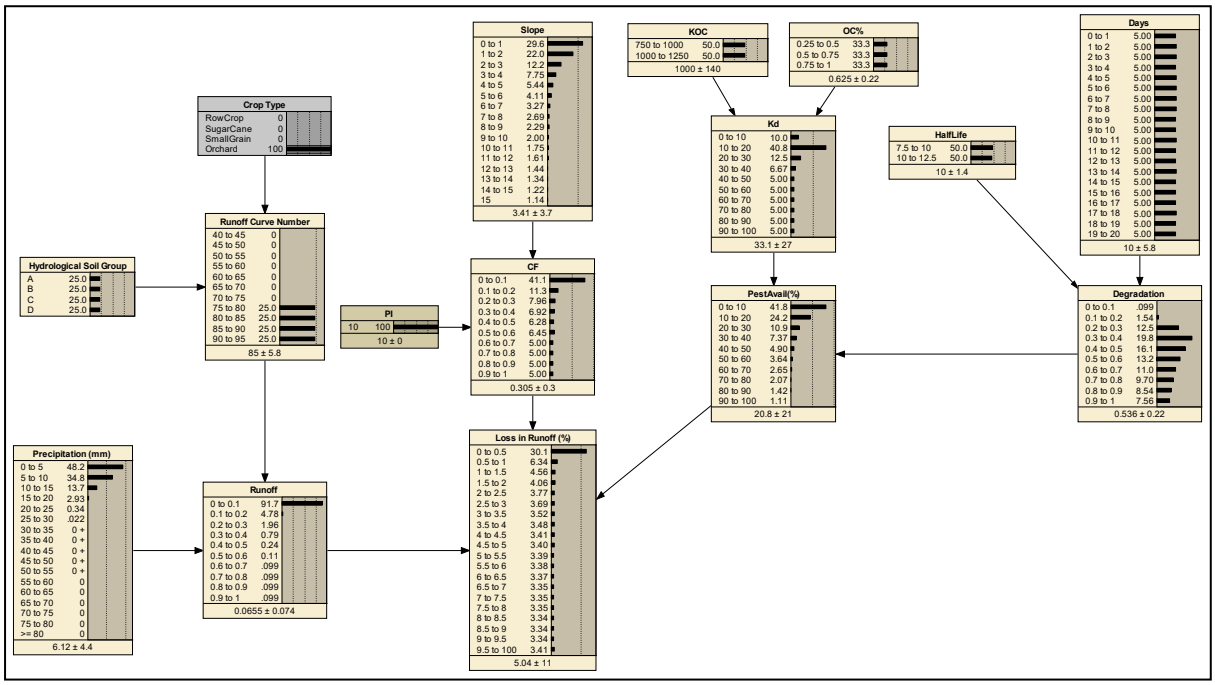


Figure 4-13 BN estimating the probability that a percentage of an applied pesticide will be lost in runoff.

# 5. Pesticide leaching potential field studies

*T Nepfumbada, M van der Laan*

## 5.1. Introduction

The South African groundwater strategy published by the Department of Water Affairs (2010) seeks to ensure that groundwater is recognized, utilized and protected as an integral part of South Africa's water resource. The groundwater strategy also highlights the fact that instances of pollution need to be addressed as soon as they are detected because it is cheaper and easier to prevent pollution than to embark on a clean-up operation after pollution had occurred. However, the strategy does not refer explicitly to agricultural activities as sources of pollution that can influence groundwater quality.

The pesticide policy document published by the Department of Agriculture Forestry and Fisheries (RSA, 2010) does, however, recognize that pesticides usage may results in adverse effects on groundwater, surface water, humans and non-target organisms. The policy proposes that future regulatory decisions be made based on assessment of the human and environmental risks posed by pesticides. The policy also seeks to introduce an effective approach to reduce pollution of water by pesticides.

In the European Union, the groundwater Maximum Allowable Concentration is set at 0.1 µg/L for any specific pesticide and 0.5 µg/L for all pesticides (London et al., 2000). This is equated to 0.1% of a typical dose of 1 kg/ha, implying that the validation status of pesticide leaching is most relevant at leaching levels of 1.0% of the dose (Vanclooster et al., 2000). The World Health Organization (WHO) has different drinking water limits for each pesticide (Zhang et al., 2009). In South Africa, groundwater monitoring studies conducted for the Water Research Commission, have established that some pesticide concentrations do occur at levels greater than 0.1 µg/L (London et al., 2000). Locally though, drinking water pesticide limits are not regularly published for all currently registered pesticides.

A lysimeter can be defined as a container loaded with soil intended to represent field environmental conditions that are used to monitor soil, water and plant interactions with the intention of studying the fate and mobility of water, pesticides, nutrients, gases, tracers, trace elements, heavy metals, metalloids, viruses, radionuclides and/or bacteria (Corwin, 2000). In more developed regions such as Europe, the use of lysimeters as an essential tool for water quality risk assessment is well-recognised (Francaviglia and Capri, 2000). No field lysimeter studies have been conducted in South Africa to simulate the leaching potential of pesticides to groundwater to the best of our knowledge, despite widespread consensus that conducting such studies is essential to better understand the fate of pesticides under local conditions.

The aim of this study was to explore the leaching potential of selected pesticides based on their physical and chemical properties using lysimeter experiments. The pesticides groups studied include triazines (atrazine and terbuthylazine), trikitones (mesotrione), chloroacetanilide (s-metolachlor), phenoxyacids (MCPA), bromoxynil and pinoxaden (phenylpyrazolin).

## 5.2. Materials and Methods

A total of four experiments were initiated in 2016. One experiment was on irrigated winter wheat and three on maize grown in summer. Winter wheat was planted in two weighing lysimeters located at the University of Pretoria's Experimental Farm, which also had a G3 Drain gauge next to them. Irrigated maize was then planted as a rotational crop on the same experiment where wheat was planted. Another experiment was conducted on one of the University of Pretoria's cylindrical cement free draining lysimeters. The fourth experiment was conducted under potatoes in the Free State Province.

### Winter wheat trial methodology

Two square weighing lysimeters installed at the University of Pretoria's Experimental Farm were used. The lysimeters are 0.9 m deep and with side lengths of 2.2 $m^2$. The design of these weighing lysimeters is similar those described in (Hutson et al., 1980). After land preparation, wheat variety PAN 3400 was planted on the 28th of June 2016. Soil samples were collected at planting from the trial site for physical and chemical property analysis and the results are listed on Table 5-1. Soil samples were collected at 0-20, 20-40 and 40-60 cm depth. The soil physical and chemical properties were analysed at Omnia laboratory which is IS017025 accredited.

Before planting the crop, nitrogen, phosphorus and potassium fertilizer was applied at recommended commercial rates. The pesticides used over the growing season are listed in Table 5-2. The pesticides chosen are those registered for wheat to control of weeds and other pests. All the pesticides used were applied as post-emergence sprays using a backpack sprayer adhering to labels recommendations. The physical and chemical properties of the pesticides used are summarized on Table 5-3. Rainfall and irrigation data over the winter season are shown in Table 5-4.

Table 5-1 University of Pretoria weighing lysimeter soil properties

| Sampling depth (cm) | 0-20 | 20-40 | 40-60 |
|---|---|---|---|
| Soil layer | Top soil | Sub-soil | Sub-soil |
| Colour code | R Br | R Br | R Br |
| Bulk density (kg/m$^{-3}$) | 1130 | 1170 | 1135 |
| pH | 5.5 | 5.5 | 5.4 |
| Exchange acidity | N/A | N/A | N/A |
| S (mg/kg$^{-1}$) | 10 | 11 | 12 |
| P (mg/kg$^{-1}$) | 27 | 21 | 21 |
| K (mg/kg$^{-1}$) | 178 | 146 | 129 |
| K(% of Exch CEC) | 9 | 8 | 7 |
| Ca (mg/kg$^{-1}$) | 663 | 600 | 639 |
| Ca (% of Exch CEC) | 63 | 62 | 64 |
| Mg (mg/kg$^{-1}$) | 182 | 171 | 175 |
| Mg (% of Exch CEC) | 28 | 29 | 29 |
| Na (mg/kg$^{-1}$) | 9 | 9 | 8 |
| Na (% of Exch CEC) | 1 | 1 | 1 |
| Exch CEC | 5.3 | 4.8 | 5.0 |
| Ca/Mg | 2.2 | 2.1 | 2.2 |
| Mg/K | 3.3 | 3.8 | 4.3 |
| (Ca + Mg)/K | 11 | 12 | 14 |
| $NO_3$-N (mg/kg$^{1}$) | 13 | 11 | 9 |
| $NH_4$-N (mg/kg$^{1}$) | 16 | 13 | 19 |
| Sand % | 64 | 57 | 58 |
| Silt % | 13 | 18 | 13 |
| Organic carbon (%) | 0.99 | 1.12 | 1.29 |
| Organic matter (%) | 1.70 | 1.93 | 2.22 |

Table 5-2 Winter wheat trial pesticide application details

| Brand Name | Active ingredient | Category/ Group | Application rate | Application date | Status |
|---|---|---|---|---|---|
| Bromotril | Bromoxynil | Herbicide | 1.0 l/ha | 02/08/2016 | Analyzed |
| Makhro MCPA | MCPA | Herbicide | 2.2 l/ha | 02/08/2016 | Analyzed |
| Axial | Pinoxaden | Herbicide | 778 ml/ha | 02/08/2016 | Analyzed |
| Pyrinex | Chlorpyrifos | Insecticide | 750 ml/ha | 12/10/2016 | Not analyzed |
| Orius | Tebuconazole | Fungicide | 750 ml/ha | 12/10/2016 | Not analyzed |

Table 5-3 Physical and chemical characteristics of the pesticides used

| Pesticide | Octanol water partition coefficient (Kow) | Organic carbon water partition coefficient (Koc) | Hydrolysis half-life (days) | Soil half-life (days) | Water solubility (mg/L 25 $^{o}$C) | Henry's Constant |
|---|---|---|---|---|---|---|
| Atrazine | 2.5 | 39-173 ml/g | 10-105 | 66-77 | 33 | 1.5 X $10^{-4}$ |
| Bromoxynil | 2.8 | 639 | 11.0 | <1.0 day) (1-34)* | 89 | 5.3 x $10^{-4}$ |
| MCPA | 2.75 (pH 1), 0.59 (pH 5 ), 0.71 (pH 7) | 110 (FAO) | 22 | 3-4 months | 0.395 (pH 1) 26.2 (pH 5) 293.9 (pH 7) 320.1 (pH 9) | 5.4 x $10^{-5}$ |
| Mesotrione | 0.11, pH 5 : 0.90, pH 7 and 9: <-1.0 (EC) | 387 | 30 | 31 | 2200 | <5.1 x $10^{-7}$ |
| s-Metolachlor | 3.05 | 121-309 | | 30 | 480 | 2.4 x $10^{-3}$ |
| Pinoxaden | 3.2 | 121-852 | Fast | <1.0 | 200 | 9.2 x $10^{-7}$ |
| Terbuthylazine | 3.21 | 162-278 | | 30-60 | 8.5 | 4.05 x $10^{-3}$ |

*Pesticide Manual Sixteen's edition 2012; European Commission: SANCO/141/2001;*US EPA, 1998b*

Table 5-4 Rainfall and irrigation data for the winter wheat trial

| Date | Irrigation | Rainfall | Date | Irrigation | Rainfall |
|---|---|---|---|---|---|
| 01-Jul-16 | 6.0 | | 03-Sep-16 | 30.3 | |
| 04-Jul-16 | 9.0 | | 08-Sep-16 | 30.3 | |
| 08-Jul-16 | 24.0 | | 16-Sep-16 | 30.3 | |
| 18-Jul-16 | 11.0 | | 20-Sep-16 | 30.4 | |
| 26-Jul-16 | | 3.1 | 21-Sep-16 | 10.4 | |
| 27-Jul-16 | 30.7 | | 27-Sep-16 | 40.4 | |
| 31-Jul-16 | 15.2 | | 02-Oct-16 | 40.4 | |
| 05-Aug-16 | 15.2 | | 07-Oct-16 | 29.7 | |
| 12-Aug-16 | 14.8 | | 11-Oct-16 | 41.1 | |
| 16-Aug-16 | 10.7 | | 15-Oct-16 | | 1.6 |
| 27-Aug-16 | 30.3 | | | | |

Both Pyrinex and Orius were applied when the crop canopy cover was very dense on the 12th of October 2016 for the control of insects and leaf diseases that occurred. Due to the lack of adequate rainfall and irrigation to facilitate leaching events as expected, only one sample per the lysimeter was collected on the 18th of August 2016. The water samples were collected at a depth of 1.0 m at the bottom of the lysimeters using 1.0 L glass bottles due to the fact that the pesticides analytical labs require a minimum volume of 750 ml for laboratory analysis. The samples were collected directly into the glass bottles at the bottom of the lysimeters. SPES20 suction cups (UMS Germany) were installed at depths of 0.15, 0.30, 0.50, 0.70 m in the two lysimeters. These are expensive, low sorption suction cups made from Teflon and can theoretically be used to be samples soil water pesticide

concentrations. Unfortunately there instruments did not sample adequately (or at all in some cases), and could therefore not be used to collect data as originally envisioned. The samples collected were stored in cold until the analyses were performed by Liquidtech Analytical Laboratory. Both chlorpyrifos and tebuconazole were not analysed because they were applied late in the season when the crop stand was very dense.

**Summer maize trial methodology**

Two experiments were set up at the University of Pretoria, one experiment was located at the same site used for the winter wheat experiment using two weighing lysimeters as described above. The other experiment was set up in the cement cylindrical free draining lysimeters filled with three different types of soil (Van der Laan, 2009). The free drainage cement cylindrical lysimeters have a volume of 6.1 $m^3$, a surface area of 4.7 $m^2$ and a depth of 1.3 m. The soils contain 11, 18 or 24% clay and a gravel layer is placed at the bottom of each lysimeter to facilitate drainage.

The maize cultivar PAN3Q240 was planted on the 8$^{th}$ of December 2016 on the weighing lysimeter's plot. On the 9$^{th}$ of December 2016 the same maize cultivar was planted on the three cement cylindrical lysimeters. Herbicides application was done on 09$^{th}$ and 12$^{th}$ of December 2016, using a backpack sprayer as pre-emergence sprays (Table 5-5). The chemicals used were donated by Agchem Africa (Cheetah = Atrazine plus terbuthylazine L 6666 and Callisto = mesotrione L6795 and Tolla Super 960 = mesotrione L9878). Both Cheetah and Callisto were applied for a second time due to volunteer wheat crop that became a weed on the two weighing lysimeter plot using the same application rates as detailed on Table 5-5. Fertilisers were applied at recommended rates. From both the weighing lysimeters and free drain lysimeters, six sampling intervals were used to collect a volume of 1 L water samples. Samples were collected directly into glass bottles at the bottom of the lysimeters and stored in the cold room at the University of Pretoria's Experimental Farm until the analyses were performed by Liquidtech Laboratory.

Table 5-5 University of Pretoria summer maize trial pesticide application details

| Brand name | Active ingredient | Category | Application rate | Application dates |
|---|---|---|---|---|
| Callisto | Mesotrione | Herbicide | 260 ml/ha | 09/12/2016 &15/12/2016 |
| Cheetah | Atrazine/terbuthylazine | Herbicide | 2.5 l/ha | 09/12/2016&15/12/2016 |
| Tolla super 960 | s-metolachlor | Herbicide | 0.4 l/ha | 09/12/2016&15/12/2016 |

**Bloemhof-Christiana G3 drain gauge maize experiment**

The trial methodology for the WRC Project K5/2501 was used for the purposes of pesticides leaching data collection (Machakaire et al., in press). The maize cultivar planted was Monsanto 78-14. The lysimeter installation had been done following the methodology outlined in Decagon G3 drain gauge manual. The G3 drain gauge installed to a 1.2 m depth from the soil surface. Maize was planted on approximately 25 ha on the 29$^{th}$ of September 2016 and irrigated with a centre pivots using river water. Soil samples were taken before the maize crop was planted and the analyses was performed by the Intertek laboratory (Table 5-6). Atrazine was applied pre-emergence at planting and both mesotrione and terbuthylazine were applied early post-emergence of the maize crop and weeds (see Table 5-7).

Table 5-6 Bloemhof-Christiana summer maize trial soil properties

| Parameter | RG3-Batch 1 | RG3-Batch 2 | RG3-Batch3 |
|---|---|---|---|
| pH | 7.01 | 5.83 | 5.99 |
| PBray 1 (mg/kg) | 16 | 5 | 4 |
| Na (mg/kg) | 30 | 26 | 27 |
| K (mg/kg) | 158 | 127 | 57 |
| Ca (mg/kg) | 289 | 331 | 417 |
| Mg (mg/kg) | 114 | 141 | 187 |
| Exchangeable acid | 0 | 0 | 0 |
| % Ca | 49.7 | 51 | 53.7 |
| %Mg | 32 | 35.6 | 39.4 |
| %K | 13.9 | 10 | 3.8 |
| %Na | 4.4 | 3.4 | 3 |
| Acid saturation | 0 | 0 | 0 |
| Ca:Mg | 1.6 | 1.4 | 1.4 |
| (Ca+Mg)/K | 5.9 | 8.7 | 24.6 |
| Mg:K | 2.3 | 3.6 | 10.4 |
| (Ca+Mg+K+Na+H) | 2.9 | 3.3 | 3.9 |
| Na:K | 0.3 | 0.3 | 0.8 |
| CEC | 2.9 | 3.3 | 3.9 |
| g/ml | 1.263 | 1.91 | 1.213 |
| mg/kg S | 12.28 | 6.94 | 12.23 |
| mg/kg $NO_3$ | 7.07 | 1.77 | 2.91 |
| Mg/kg $NH_4$ | 0.02 | 0.01 | 0.01 |
| % Clay | 6 | 10 | 12 |
| % Silt | 1.96 | 4.64 | 3.56 |
| % Sand | 92.04 | 85.36 | 84.44 |
| % C | 0.01 | 0.03 | 0.02 |

Table 5-7 Summer Maize Experiment (Christiana)

| Active ingredient | Category | Application rate |
|---|---|---|
| Atrazine | Herbicide | 2.5 l/ha |
| Mesotrione | Herbicide | 260 ml/ha |
| Terbuthylazine | Herbicide | 2.0 l/ha |

## 5.3. Pesticide Analyses

### Extraction

Analytes were extracted from the water samples using C18 solid phase extraction. Cartridges were equilibrated with 6 mL pure MeOH. After equilibration, samples were loaded at a flow rate of approximately 6 mL/min. After samples were loaded, cartridges were washed with 6 mL of ultrapure water. Extracts were eluted into 6 mL tubes using 2 mL of MeOH and 2 mL of acetonitrile. Eluates were evaporated using a Savant SC 210A Speedvac concentrator with a Thermo RVT 4104 refrigerated vapour trap. Extracts were reconstituted in 500 uL of $H_2O$ / 7.5 mM ammonium formate.

### Analyses

Samples were analysed using a Sciex 4000QTRAP hybrid triple quadrupole ion trap mass spectrometer with a Shimadzu LC20AB HPLC stack as a front end. All data acquisition and processing was performed using Analyst 1.5 (Sciex) software.

Twenty microliter of each extracted sample was separated on a C18 (150 x 2 mm, Luna 5 µ Phenyl-Hexyl, Phenomenex) column at a flow rate of 300 uL/min starting at 5% mobile phase B (MeOH/ 7.5 mM ammonium formate), at 1 min ramping up to 95% B over 1 min and staying there for 3 minutes, before re-equilibrating the column at 5% B for 5 minutes. Eluting analytes were analysed in separate LC runs in both positive and negative ionization modes using a targeted multiple reaction monitoring (MRM) workflow. The targeted analyses were performed using 2 MRM transitions per analyte.

During a multiple reaction monitoring (MRM) scan type the instrument is used in triple quadrupole mode where every ionised analyte (the precursor) eluting off the column is fragmented in the collision cell to produce fragment masses. A set of masses, the precursor mass and one fragment mass constitutes a transition. The instrument jumps between different transitions in an MRM transition list during an analysis cycle, with each cycle typically lasting a 1 second. If a transition is detected the instrument's response is registered and a chromatogram is generated. The peak area on the chromatogram generated from the first and most sensitive transition was used as the quantifier while the second of the transitions are used as a qualifier. The qualifier serves as an additional level of

confirmation for the presence of the analyte, the retention time for these 2 transitions needs to be the same.

The source dependant parameters were: curtain gas: 20 psi, electrospray voltage: 5500V, collision gas: high, source temperature: 400°C, ionisation gas: 30 psi, heater gas: 30 psi. The source dependant parameters for the negative ionising analytes were: curtain gas: 20 psi, electrospray voltage: 4500V, collision gas: high, source temperature: 400°C, ionisation gas: 30 psi, heater gas: 30 psi.

A 4 point external calibration curve was constructed ranging from 0.0005 ppb to 0.5 ppb by spiking 500 mL of laboratory water with the analytes at the correct concentration and extracting them by SPE as described above. All curves had linear range with an $r^2$ fit value of 0.95.The ion source used an ion spray voltage setting of 5500 V, 500$^{o}$C heater temperature to evaporate excess solvent, 50 psi nebuliser gas, 50 psi heater gas and 25 psi curtain gas. Samples were submitted into batches that include solvent blank runs between each sample analysed. The lowest limits of quantification (LOQ) were 0.0005 µg/L for atrazine, metolachlor, pinoxaden and terbuthylazine and 0.0050 µg/L for bromoxynil, MCPA and mesotrione.

## 5.4. Results

Pesticides analytical results for the winter wheat and summer maize trials are presented in Tables 5-8 to 5-14. Most of the pesticides were detected at levels below the EU groundwater limit of 0.1 µg/L, except for MCPA, which was detected above the EU concentration threshold in weighing lysimeter 1 in the winter wheat trial. In the Bloemhof-Christiana maize trial, metolachlor was detected at a concentration significantly higher than the EU groundwater limit in the first three sampling events, but on the last sampling event, the concentration decreased to a level below the EU limit.

Table 5-8 University of Pretoria winter wheat trial

| Location | Sampling Date | Active ingredients analyzed | Concentration µg/l |
|---|---|---|---|
| UP-Weighing Lysimeter 1 | 18/08/2016 | Bromoxynil | 0.0206 |
| | | MCPA | 1.0300 |
| | | Pioxaden | ND |
| UP-Weighing Lysimeter 2 | 18/08/2016 | Bromoxynil | <LOQ |
| | | MCPA | 0.0927 |
| | | Pioxaden | ND |

*ND = Not detected*

Table 5-9 University of Pretoria summer maize trial − weighing lysimeter 1

| Date | Atrazine | Bromoxynil | MCPA | Mesotrione | Metolachlor | Pinoxaden | Terbuthylazine |
|---|---|---|---|---|---|---|---|
| 22/11/2016 | - | - | - | - | - | - | - |
| 14/12/2016 | - | - | - | - | - | - | - |
| 29/12/2016 | 0.0180 | ND | 0.0064 | ND | 0.2940 | ND | 0.0330 |
| 08/01/2017 | 0.0076 | ND | 0.0064 | 0.0052 | 0.0026 | ND | 0.0026 |
| 16/02/2017 | 0.0096 | ND | 0.0051 | ND | 0.0051 | ND | 0.0128 |
| 22/02/2017 | - | - | - | - | - | - | - |

*(- = No drainage and ND = Not detected)*

*NB: Pinoxaden, Bromoxynil and MCPA were applied on the same site in August 2016 in the Winter Wheat Experiment*

Table 5-10 University of Pretoria summer maize trial − weighing lysimeter 2

| Date | Atrazine | Bromoxynil | MCPA | Mesotrione | Metolachlor | Pinoxaden | Terbuthylazine |
|---|---|---|---|---|---|---|---|
| 22/11/2016 | 0.0140 | ND | ND | 0.0036 | 0.0147 | ND | 0.00286 |
| 14/12/2016 | 0.0218 | <LOQ | 0.0067 | ND | 0.2960 | ND | 0.0228 |
| 16/12/2016 | 0.0013 | ND | ND | ND | 0.0015 | <LOQ | 0.0020 |
| 08/01/2017 | 0.0027 | ND | ND | 0.0051 | 0.0028 | ND | 0.0039 |
| 16/02/2017 | - | - | - | - | - | - | - |
| 22/02/2017 | 0.0042 | ND | ND | ND | 0.0039 | ND | 0.0044 |

*(- = No drainage and D = Not detected)*

Table 5-11 University of Pretoria summer maize trial − cylindrical lysimeter 1

| Date | Atrazine | Mesotrione | Metolachlor | Terbuthylazine |
|---|---|---|---|---|
| 10/01/2017 | ND | ND | ND | ND |
| 17/01/2017 | ND | ND | ND | ND |
| 24/01/2017 | ND | ND | 0.0009 | ND |
| 28/01/2017 | ND | ND | 0.0009 | ND |
| 02/02/2017 | ND | ND | 0.0010 | ND |
| 24/02/2017 | ND | ND | 0.0007 | ND |

*(ND = Not detected)*

Table 5-12 University of Pretoria summer maize trial − cylindrical lysimeter 2

| Date | Atrazine | Mesotrione | Metolachlor | Terbuthylazine |
|---|---|---|---|---|
| 10/01/2017 | 0.0010 | ND | 0.0011 | 0.0015 |
| 17/01/2017 | - | - | - | - |
| 24/01/2017 | - | - | - | - |
| 28/01/2017 | - | - | - | - |
| 02/02/2017 | - | - | - | - |
| 24/02/2017 | ND | ND | ND | ND |

*(- = No drainage and D = Not detected)*

Table 5-13 University of Pretoria summer maize trial − cylindrical lysimeter 2

| Date | Atrazine | Mesotrione | Metolachlor | Terbuthylazine |
|---|---|---|---|---|
| 10/01/2017 | ND | ND | ND | ND |
| 17/01/2017 | ND | ND | ND | ND |
| 24/01/2017 | ND | ND | ND | ND |
| 28/01/2017 | ND | ND | ND | ND |
| 02/02/2017 | ND | ND | ND | ND |
| 24/02/2017 | ND | ND | ND | ND |

*(- = No drainage and D = Not detected)*

Table 5-14 Chrisitiana-Bloemhof summer maize trial

| Date | Atrazine | Mesotrione | Terbuthylazine |
|---|---|---|---|
| 24/11/2016 | 0.0132 | 0.0306 | 0.0135 |
| 08/12/2016 | 0.0117 | 0.0371 | 0.0108 |
| 02/02/2017 | 0.0253 | 0.0364 | 0.0106 |
| 16/02/2017 | 0.0164 | 0.0248 | 0.0040 |

The soil in the winter wheat weighing lysimeter experiment on the University of Pretoria Experimental site had 60% sand and organic matter content of between 1-2%, and the pH of between 5.4 and 5.5. Under these conditions all herbicides studied did not show any leaching tendencies, although it is acknowledged that irrigation was very carefully scheduled according to crop demand. However, it is difficult to conclude why excessive leaching did not happen in the sandier soils which contain 94-96% sand in the Bloemhof-Christiana experimental site where atrazine, mesotrione and terbuthylazine were applied. Bromoxynil octanoate quickly break downs to bromoxynil phenol through hydrolysis with a half-life ranging from one day up to 34 days, and therefore, does not generally persist in the environment (US EPA, 1998a). Hiller et al. (2010) reported that MCPA had a significant potential to contaminate groundwater when applied in sandy soils with low organic matter and higher water infiltration rate.

In the University of Pretoria cylindrical lysimeters only s-metolachlor was observed to leach at 1.3 m whereas the other herbicides tested such as atrazine, mesotrione and terbuthylazine were not detected in the water samples collected, and this could be attributed to physical and chemical properties of the soils used. Sakaliene et al. (2007) indicated that alachlor, amitrole, atrazine, dicamaba, imazamox, imazethapyr, pendimethalin and simazine were predicted to show reduced leaching potential in soils with higher clay content. If a pesticide has a higher Koc value, then it would be strongly sorbed to the soil and therefore made less mobile (Tiryaki and Temur, 2010). Due to its low Koc of 200 ml/g and high water solubility of 530 mg/l, metolachlor could be leached to deeper soil layers (Francaviglia and Capri, 2000). The results recorded in this study for bromoxynil, mesotrione, pinoxaden and terbuthylazine are similar to the European Food Safety risk assessment conclusions (EFSA, 2017, 2016, 2013 and 2011) in the sense that, these substances did not leach at concentrations above the EU drinking water limit of 0.1 (µg/l). However, it should be noted that no metabolites were analysed in this study due tohigh cost associated with the analysis.

## 5.5. Conclusions

Pesticide leaching potential has been measured for the first time under field conditions for South African maize and wheat cropping systems. For some pesticides, leaching concentrations were above the EU threshold of 0.1 µg/L. Even for those that were observed to leach at concentrations below the threshold, risk to the environment still exists, however. It is important to note that daughter metabolites were not measured, and these too can pose a risk to the environment.
The fairly new Decagon G3 drainage gauges proved very useful to measure pesticide leaching, and further application of these devices in leaching studies is encouraged. The expensive SPES20 suction cups did not perform well under our trial conditions and are therefore not recommend for application in research under similar conditions.

Further value can be added to these leaching data by using the drainage fluxes to estimate the loads of pesticide leached from fields. These data can also be extremely useful for the calibration and validation of pesticide leaching models.

# 6. Exposure Scenarios

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## 6.1. Introduction

The exposure characterisation describes the potential for a plant or animal to come into contact with a pesticide for the purpose of risk assessment. Furthermore, the exposure assessment should be able to describe exposure pathways (i.e. routes of transport).The exposure assessment typically considers the most important transport routes for pesticides entering surface waters. Runoff is considered the most important route of entry for pesticides (Schulz, 2001b) and as such, in terms of exposure assessment scenario it is important to include environmental parameters that influence movement of water from agricultural field to surface water resources. Surface runoff occurs when the precipitation rate exceeds the infiltration rate of the soil or when the length of a rainfall event exceeds the infiltration capacity of a soil. A complex interaction of a multiple number of environmental variables ultimately influences the quantity of pesticide that can be expected to be present in surface runoff, the most important of which include rainfall event, antecedent soil water content, the slope and the soil types of the catchment, pesticide interception by the crop as well as the size and characteristics of vegetated buffer strips (Cole et al., 1997).

Rainfall is the main source of runoff because runoff cannot occur without the rainfall event (except if irrigation water is applied in such a way as to lead to runoff). Runoff is generated by rainfall events and its occurrence and quantity are dependent on the characteristics of the rainfall event (i.e. intensity, duration and distribution). The quantity of pesticides that can be expected to be present in surface runoff is dependent on the interval between the application of pesticides and the rainfall event. Studies have shown that the first heavy rainfall after application results in the highest quantity of pesticides in surface waters (Dabrowski et al., 2002a; Domagalski et al., 1997). Large rainfall events occurring a few days after the application of pesticides have resulted in very high concentrations of pesticides being detected in the Lourens River (Schulz, 2001a).Slope has also been shown to be a key factor influencing runoff but can be greatly modified by the presence of vegetation (Wilcox and Wood, 1989).

Soil properties are also a vital influence in terms of the amount of surface runoff and the quantity of transported pesticide that occurs during an event. Soils with higher organic carbon content have the tendency to bind pesticides more than soils with low organic carbon content (Flury, 1996), while for any particular precipitation amount, loamy and clay soils contribute a greater quantity of surface runoff (and hence pesticide loss) than sandy soils, which promote infiltration and leaching . Soils with high soil moisture content are more prone to runoff losses than drier soils.

Crop types and their pesticide interception capacity also influence the amount of pesticides available for runoff because when more pesticides are intercepted by leaves and stems, then less pesticide reaches the soil surface. Furthermore, there are different quantities of pesticides applied to different crops. For example, high quantities of pesticides are applied to maize compared to lower quantities applied to avocadoes (GfK Kynetec (2009)). Also, different crops in combination with crop-specific growing phases have varying pesticide interception capacity. This means a fully grown orange tree intercepts a larger fraction of pesticides than a fully grown maize crop, the same applies when these crops are still small compared to when they are fully matured.

As highlighted above there are a number of weather, soil and other geographical factors that influence the transport of pesticides in the environment. These factors vary widely from one catchment to another in the country. Furthermore simulation models are often complex and require large numbers of input parameters and as a result are difficult to use properly. From a modelling viewpoint it is therefore difficult to account for and incorporate the high degree of natural variation in all of these input parameters when performing exposure assessments. To simplify this process a recognised approach is used to identify relevant standardized exposure assessment scenarios that represent typical environmental conditions under which pesticides may be applied. The primary purpose of defining standard scenarios is to increase the consistency with which industry and regulators predict pesticide exposure in surface waters. Having standard scenarios means that the user has less input to specify, and appropriate guidance simplifies the selection of these inputs. Worst case scenarios are desirable in that it represents a conservative estimate of pesticide exposure.

In the EU, ten different scenarios have been developed for use as data input into modelling, which are representative of typical environmental conditions in major agricultural production areas (FOCUS, 2001). These scenarios consider all relevant entry routes to a surface water body (e.g. runoff) as well as all appropriate target groups, surface water situations, topography, climate, soil type and agricultural management practices. These scenarios are representative of a combination of worst-case situations in which off-target movement of pesticides would be expected to be highest. For example, agricultural areas experiencing high annual rainfall with steep slopes and soils with high clay content demonstrate characteristics that would lead to relatively high pesticide runoff. These areas can be considered to be representative of worst case runoff conditions and a favourable risk assessment derived using input data from these areas (for the exposure assessment) would therefore be protective of aquatic ecosystems in all agricultural areas (for runoff as a transport route). The use of worst-case scenarios therefore avoids the need to perform runoff simulations in areas where pesticide inputs associated with runoff would be expected to be relatively low, which significantly reduces the burden on modelling effort.

Existing models for pesticide entry into streams via runoff include CREAMS (Kniesel, 1980) or PRZM (Carsel et al., 1984), which were reviewed by the Forum for the Coordination of Pesticide Fate Models and their Use (FOCUS) (Adriaanse et al., 1997). These complex models reflect the number of

different factors that influence the fate and transport of a pesticide at a field scale. Data requirements typically required for running these models are those that influence the fate and transport of pesticides in the environment.

## 6.2. Environmental parameters that influence runoff

There are number of different environmental parameters that influence the fate and transport of pesticides at field scale. An interaction of these parameters ultimately influences the quantity of pesticide that can be expected to be available for surface runoff. These parameters vary from one geographical area to the other and are described below:

### Rainfall

Rainfall and other forms of precipitation occur when warm moist air cools and condensation occurs. Since warm air can hold more water than cool air, when the warmer air is cooled the moisture condenses to liquid and eventually it rains. The following are three types of rainfall that occur in various geographical areas of South Africa (Climatology and Meteorology, 2017; Weather and Climate, 2017).

Convection rainfall: This type of rainfall occurs due to thermal convection as a result of heating of the ground surface. When the land warms up, it heats the air above. This causes the air to expand and rise. As it rises it cools and excess water contained in the air condenses. If this process continues then rain will form. The following preconditions must exist for this type of rainfall to occur.
Abundant supply of moisture through evaporation to air so that relative humidity becomes high and intensive heating of the ground surface through incoming shortwave electromagnetic solar radiation. This type of rainfall occurs for a short period of time but in the form of heavy showers.

Orographic or relief rainfall: This is the type of rainfall which occurs when air has blown over the sea and is then being forced up over an area of high topography. This causes air to cool and moisture in the air to condense into rainfall. The preconditions for formation of orographic rainfall are:
There should be a mountain barrier across the wind direction, so that the moist air is forced on obstruction to move upward. There should be sufficient moisture in the air. The mountain must be high enough to block the incoming moist air. Once over the top of the mountain the air will usually drop down the other side, warming as it does so. This means it has a greater ability to carry water moisture and so there is little rain on the far side of the mountain. This area is called the rain shadow.

Cyclonic or frontal rainfall: The type of rainfall occurs when warmer air is forced to rise over cold air. The moist warm air condenses as it cool which creates clouds and rain. Frontal rain produces a variety of clouds, which bring moderate to heavy rainfall.

South Africa experiences a high degree of rainfall variability of which it is about half of the global average. Rainfall increases from west to east and with semi-desert regions in the north-west. While the Western Cape has a Mediterranean climate with winter rainfall, most of the country experiences summer rainfall. The seasonal rainfall regions are described below (South African Weather and Climate, 2017):

The winter rainfall region: Winter rainfall occurs only in the southwestern part of the country, particularly around the Cape Town (South African Weather and Climate, 2017). It stretches more or less from the mouth of the Olifants River (north-west) to the mouth of the Breede River (south). Overall, the Western Cape climate is typically Mediterranean with warm, dry summers and mild, moist winters and low summer rainfall prevail.

Summer rainfall region: Rainfall in the country generally occurs during summer (November through March) and it varies considerably from west to east (South African Weather and Climate, 2017). In the northwest part of the country, annual rainfall often remain below 200 mm. in contrast, much of the eastern Highveld receives 500 mm to 900 mm of rainfall per year and occasionally exceeds 2000 mm. A large area of the centre of the country receives about 400 mm of rain (on average).

A rain gauge is an instrument used by meteorologists and hydrologists to gather and measure the amount of liquid precipitation over a set period of time (South African Weather Service, 2017). The rain accumulated in the bucket of the rain gauge is poured into a specially calibrated measuring glass and the millimetre reading is recorded, where after the water is discarded. The rainfall measured between 08:00 South African Standard Time (SAST) yesterday and 08:00 SAST today is recorded against yesterday's date on the database. What is meant by 1 mm of rainfall is rainfall equivalent to 1 litre of water in a 1 square meter box with no runoff, infiltration or evaporation.

The South African Weather Service also has a number of electronic rain gauges called tipping bucket rain gauges. These gauges consist of a large cylinder set into the ground or hung from a mast. At the top of the cylinder is a funnel that collects and channels the precipitation. The precipitation falls into one of the two small buckets which are balanced side by side. As soon as it starts raining one of the buckets fills with water. After an amount equal to 0.2 mm falls into the bucket the bucket tips and an electrical signal is sent to a logger. The next bucket is then in place to collect precipitation. The two buckets seesaw up and down collecting and recording the rainfall. The instrument is thus able to record not only the amount of rain that falls but also records intensity of the rainfall (South African Weather Service, 2017).

**Soil**

Soil is the unconsolidated mineral or organic material on the immediate surface of the earth that serves as a natural medium for the growth of land plants (USDA, 2018). Soils have different types of properties including texture, structure, water holding capacity and pH (Schoonover and Crim, 2015). These properties combined make soils a useful resource for a wide range of purposes. Soil properties govern what type of plants grows in a soil or what particular crops grow in a region. Below are some of the vital physical, chemical and biological factors that determine the soil properties and quality (Schoonover and Crim, 2015; SSC107-Fall, 2000):

Soil texture: Soil is made up of different sized particles. Soil texture refers to the size of the particles that make up the soil and it depends on the proportion of sand, silt and clay-sized particles and the organic matter in the soil (Rice, 2002). The amounts of sand, silt, clay and organic matter in a particular soil play a large part in the way that it behaves how it can be managed and what it can be used to grow (Schoonover and Crim, 2015). Sandy soils are easy to break up with a hoe (cultivate) but tend to hold little water and are characterised by dryness, whereas clay soils are more difficult to cultivate, hold a lot of water and can become waterlogged.

Soil structure: Soil structure is a key factor in the functioning of soil, its ability to support plant and animal life and moderate environmental quality with particular emphasis on soil carbon sequestration and water quality. The structure of the soil is determined by the way in which sand, silt and clay particles are clumped together (Six et al., 2000). Organic matter (decaying plants and animals) and soil organisms such as earthworms and bacteria influence soil structure. Clays, organic matter and materials excreted by soil organisms bind the soil particles together to form aggregates. Soil structure is important for plant growth, regulation of air and water movement, root development influence and nutrient availability (Lai, 1991). Good quality soil soils are friable and have fine aggregates so the soil breaks up easily if you squeeze. Poor soil structure, for example, looks different because it has been compacted and has its structure and porosity altered.

Soil chemistry: Soils can be acidic, alkaline or neutral. Soil pH influences nutrient absorption and plant growth (USDA, 2018). Some plants, like potatoes grow best in a more acidic soil (pH of 5.0-6.0). Carrots and lettuces prefer soils with a neutral pH of 7.0. Soils can become more acidic over time as minerals are leached away. Lime is often added to soil to make it less acidic. Clays and organic matter in the soil carry negative charges. Water in the soil dissolves nutrients and other chemicals. Some plant nutrients and metals exist as positively charged ions or cations in the soil environment (USDA, 2018). Among the more common cations in the soil are hydrogen (H+), aluminium (Al+3), calcium (C+2), magnesium (Mg+2) and potassium K+). Some of these nutrients and cations have positive charges, therefore they are attracted to the negatively charged organic and mineral matter, and this prevents them from being lost through leaching as water moves through the soil. Nitrate has a negative charge so it is not protected from leaching in most soils.

Soil properties are measured as follows:

Soil texture: According to Bowman and Hutka (2002), particle size analysis (PSA) is a reliable technique used to measure each particle size group (i.e. sand, silt and clay). The technique eliminates factors that may affect the field texture such as organic matter content, clay mineralogy, cation composition and the presence of cementing agents. The PSA method include two parts, i.e. dispersion of the soil and separation of the particles into size groups. During pre-treatment stage, salts such as gypsum and organic matter, iron oxides, calcium carbonate as well as magnesium are removed. Fractionation is achieved by allowing the soil particles of different size to settle out of a solution at different times (small clay particles take long time to settle out). The fractions are eventually dried out and weighed as such sand, silt and clay must add up to 100%. Other calculations needed for this method include the use of scaling factor for pipette analysis and calculation for the sieve analysis.

Soil chemistry: Soil pH is a measure of the amount of hydrogen ion (H+) concentration that is present in soil solution (USDA, 2018). It is an indication of the acidity or alkalinity of a soil. A pH value of 7 is considered neutral, where H+ and OH- are equal both at a concentration of 10-7 moles /litre. The cation exchange capacity (CEC) of a soil is a measurement of the magnitude of the negative charge per unit weight of soil or the amount of cations a particular sample of soil can hold in an exchangeable form (USDA, 2018). The greater the clay and organic matter content, the greater the CEC should be although different types of clay minerals and organic matter may vary in CEC.

**Slope**

Slope is a surface of which one end is at a higher level than another; a rising surface or a falling surface (Cambridge Dictionary, 2018). The slope (the most widely used topographic measurement) influences the flow rates of water and sediment by controlling the rate of energy or power available to drive the flow. Steep slopes contribute to higher flow rates and more power to drive the flow than gentle slopes.

A digital elevation model (DEM) is a raster-based data structure that stores elevation values which can represent the land surface without the heights of land cover (i.e. digital terrain model) or it can represent terrain and land cover height (digital surface model) (Van Niekerk, 2016).

### Crop production

According to Crop Agriculture (2018), a crop is a plant or plant product that can be grown and harvested extensively for profit or subsistence. By use, crops fall under six categories: food crops, for human consumption (e.g. wheat, potatoes); feed crops, for livestock consumption (e.g. oats, alfalfa); fibre crops, for cordage and textiles (e.g. cotton, hemp); oil crops, for consumption of industrial uses (e.g. cotton seed, corn); ornamental crops for landscape gardening (e.g. dogwood, azalea) and industrial and secondary crops for various personal and industrial uses (e.g. rubber and tobacco). According to FAOSTAT (2008), South Africa is one of the producers of several crops which include chicory roots, grapefruit, cereals, maize, castor oil seed, pears, sisal, fibre crops. Grains and cereals are important crops in the country occupying about 60% of hectarage under cultivation in the 1990s. Maize, the country's most important crop is a dietary staple food, a source of livestock feed and an export crop. Maize production exceeds 10 million tons in good years (DAFF, 2016b). Other small grains are grown in localised areas of South Africa. For example, sorghum which is native to southern Africa is grown in parts of the Free State, as well as in the North-West and Limpopo Province. Barley is also grown primarily in the Western Cape. Pineapples are primarily grown in the Eastern Cape and KwaZulu-Natal. Tropical fruits such as bananas, avocados and mangoes are also grown particularly in the northeast and some coastal areas (DAFF, 2016b). Sugarcane is an important export crop that is cultivated in Natal and also in Mpumalanga where irrigation is used when rainfall is inadequate.

### Plant interception

Interception refers to precipitation or any form of liquid sprinkle (i.e. pesticide application) that does not reach the soil surface but it is instead intercepted by the leaves and branches of a crop. This occurs when the pesticide is captured or trapped by the canopy of a crop and eventually evaporates from the leaves and branches. The fraction of pesticide that is not intercepted will fall as a throughfall or stemflow to the soil surface. The interception depends on the leave area index (or canopy cover) and architecture of the leaves. Furthermore, a more mature crop will generally intercept a larger fraction of pesticide compared to a still-developing crop.

Linders et al. (2000) published data for growth specific interception of applied pesticides by various target crops. Though this data is unavailable in South Africa, interception data for crops such as maize, potatoes, onions, peas, etc. can still be applied.

## 6.3. How environmental parameters influence runoff

Runoff has been shown to be a major non-point source of pesticides to surface waters in agricultural areas and it is dependent on the application, environmental fate properties of pesticides and catchment-specific variables (Kuivila and Foe, 1995; Schulz, 2001a; Schulz, 2001b). These catchment variables influencing runoff include, slope, soil type, crop type and the size of the cropped

area, rainfall, density of buffer strips that lie between agricultural lands and water bodies (Cole et al., 1997).

### Rainfall

Rainfall is the key driver of hydrological processes on the environment and categorising the rainfall variability and processes of runoff generation lead to better understanding of ecosystem functioning of the catchments and its hydrology (Truncoso et al., 2016; Jarihani et al., 2017). During rainfall, horizontal flow of water occurs over the land surface (i.e. runoff). Runoff occurs when the rainfall rate exceeds the infiltration rate of the soil or when the duration of rainfall event exceed the infiltration capacity of the soil. Large rainfall events are directly linked with the majority of runoff generation and erosion. However, rainfall-runoff relationship differs from one catchment to the other. For instance, the annual rainfall required to trigger runoff in the Keelbottom catchments was higher than in the Basalt catchment (Jarihani et al., 2017). This could be attributed to vegetation cover in each catchment because the more heavily vegetated savanna catchments require more antecedent rainfall to generate runoff than in drier, poorly vegetated catchment. In addition, differences in soil texture, erosion rills and slope can also play a role.

The transport of pesticides from cultivated fields to adjacent surface waters generally occurs through runoff induced by rainfall. Runoff has been shown to be a major non-point source of pesticides to surface waters in agricultural areas (Schulz, 2001b; Dabrowski and Schulz, 2003). The time period between application and rainfall also contribute to the quantities of pesticides that enter the surface waters via rainfall-induced runoff (Schulz et al., 2001b).

### Slope

Investigations on runoff have shown that steep slope yield more runoff than gentle slopes (Dabrowski et al., 2002a; Wilcox and Wood, 1989; Dabrowski et al., 2002b). It has been shown that higher in-stream concentrations of pesticides are associated with several factors including steeper slopes in combination with loamy soils (Cole et al., 1997). In addition, the quantity of runoff may decrease with increasing slope length (Lal, 1983 quoted from Lal, 1988). This means that the water may be exposed for longer duration to infiltration and evaporation before it reaches the measuring point. The same applies when the catchment areas of different sizes are compared. Studies have shown that steeper agricultural field slopes are associated with higher amount of pesticides or regular occurrence of pesticides in the adjacent surface water resources (Dabrowski et al., 2002b; Wilcox and Wood, 1989; Probst et al., 2005). The impact of slope can also be greatly modified by the presence of vegetation (buffer strips), though erosion rills can decrease the efficiency of this vegetation to trap runoff (Stehle et al., 2016).

### Soil properties

Soil properties are also a key factor in determining the amount of water available for surface runoff during the rainfall event. More water is susceptible to runoff on loamy soils while more infiltration occurs in sandy soils. Hussein et al. (2000 concluded that soil physical properties like texture and drainage conditions of the subsoil as well as slope gradient have a vital influence on the quantity of runoff. Rainfall up to 70 mm produced more runoff on moderate slopes (10%) with heavy clay soils than on steep slopes (50%) with a sandy soils texture (Baumann et al., 2008). The extent of pesticides adsorption to soil depends on the nature and properties of soil (Dabrowski and Schulz, 2002). Clay and loamy soils are associated with higher organic carbon which tends to bind more pesticides than sandy soils. As a result, more clay and loamy soils are highly likely to generate more runoff (with dissolved pesticides) and cause more erosion (adsorbed pesticides) to the receiving waters while sandy soils promote infiltration.

### Crop types

South Africa is the largest user of pesticides in sub-Saharan Africa and wide variety of crops are produced in the country (Dabrowski et al., 2014). A large variety of pesticides are applied in significant amounts to various crops in different geographical areas in the country. Crop-specific pesticide use data is available, thus it is possible to identify the priority pesticides that are applied to many crops. Linking priority pesticides to specific crops produced in South Africa gives an indication of which area or communities are at risk of pesticides exposure. For instance, in South Africa high quantities of pesticides were applied to maize (approx. 5 000 000 kg/year), wine grapes (approx. 2 900 000 kg/year), citrus (approx. 1 400 000 kg/year), sugarcane (approx. 1 100 000kg/year) and potatoes (approx. 1 300 000 kg/year) in 2009 (Gfk Kynetec, 2009). Furthermore, Kreuger (2009) linked the amount of applied pesticides with in-stream concentration for a seven year period. According to Kreuger (2009), the total amount of pesticides lost in stream flow each year varied between 0.5 and 2.8 kg, corresponding to approximately 0.1% of the applied amount. Single pesticides losses in stream were generally less than approximately 0.3% of the applied amount during individual years.

### Plant interception

One of the crucial aspects of exposure assessment is the interception of an applied pesticide by target crop, as this determines what proportion of the applied substance remains on the leaves and stems of the plant and what proportion reaches the soil surface. A data of this nature is not available in South Africa. However, this data is available in other countries such as the Netherlands and Germany. In addition, growth-phase specific interception factors for a number of crops have been published (Linders et al., 2000). The higher the fraction of pesticide that reach the soil surface during application (i.e. fraction of pesticide that is not intercepted by the crop), the more chance of pesticide to runoff to adjacent surface water resources. As a result high amount of pesticide are expected to

occur in the surface water resource. Therefore, herbicides are more susceptible to reach adjacent water resources (compared to insecticides and fungicides) as they are intentionally applied closer to the soil surface because the targeted weed is on the ground. This is important for the purposes of performing exposure assessments in risk assessment and these factors are based on measured data for a number of crops throughout Europe and North America.

## 6.4. Classification of key environmental parameters

### Rainfall

South Africa is regarded as a semi-arid country with a mean annual rainfall of approximately 497 mm (60% of the world average), of which 65% of the country receives less than 500 mm per year (DWAF, 1994) The country is characterised by three major zones, namely the winter rainfall region of the western, south-western and southern Cape; the bimodal rainfall region of the Eastern Cape and the strong summer rainfall of the central Highveld and KwaZulu-Natal. There is wide regional variation of rainfall from west to east (Figure 6-1). In the northwest (near the border of Namibia), annual rainfall often remains below 200 mm while the eastern Highveld receives between 500 and 900 mm of rainfall annually (on few occasion it exceed 2000 mm). However, about 28% of the country receives more than 600 mm (Table 6-1).

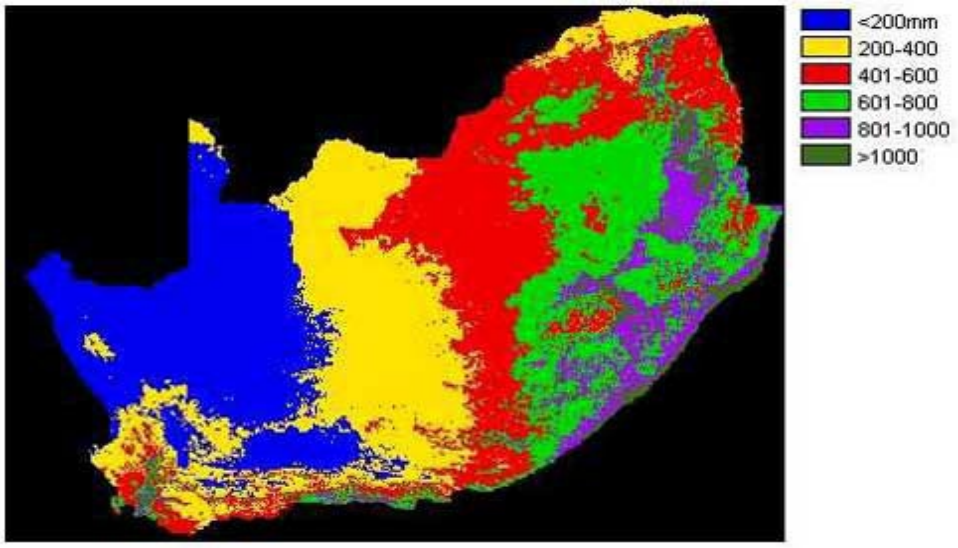



Figure 6-1 Median annual rainfall for South Africa (Dent et al., 1987).

Table 6-1 Annual rainfall distribution and climatic classification in South Africa

| Rainfall (mm) | Classification | Land surface percentage |
|---|---|---|
| <200 | Desert | 22.8 |
| 201-400 | Arid | 24.6 |
| 401-600 | Semi-arid | 24.6 |
| 601-800 | Sub-humid | 18.5 |
| 801-1000 | Humid | 6.7 |
| <1000 | Super-humid | 2.8 |

Schulze, 1997

**Slope**

Table 6-2 indicates the description of different slopes based on their percentage. The 0-3% gradient of slope generates less runoff compared to higher gradient slope such as 4-9% gradient slope, etc. Higher slopes (i.e. moderate, steep, extremely steep slopes) results in higher exposure of pesticides in adjacent surface water resources.

Table 6-2 Description of slope classes.

| Class | Description |
|---|---|
| Little | 0-3% gradient |
| Gentle | 4-9% gradient |
| Moderate | 10-15% gradient |
| Steep | 16-30% gradient |
| Extremely steep | 31-60% gradient |
| Excessively steep | >60% gradient |

*Agriculture and Agri-Food Canada, 2017*

**Soil**

Different soil types have particle sizes that range between 2 mm to <0.002 mm (Figure 6-2). For example, the particle size for clay is less than 0.002 mm, for silt it is between 0.002 and 0.075 mm and sand it is between 0.075 and 2 mm. All these soil types have different infiltration rates and generate different amounts of runoff (Table 6-3). Runoff and infiltration rates have negative correlation e.g. (sandy soils allow higher infiltration leading to less runoff while with clay soils it is the opposite). Clay to loamy soils increase the potential of pesticides exposure through runoff compared to sandy soils which promote infiltration.

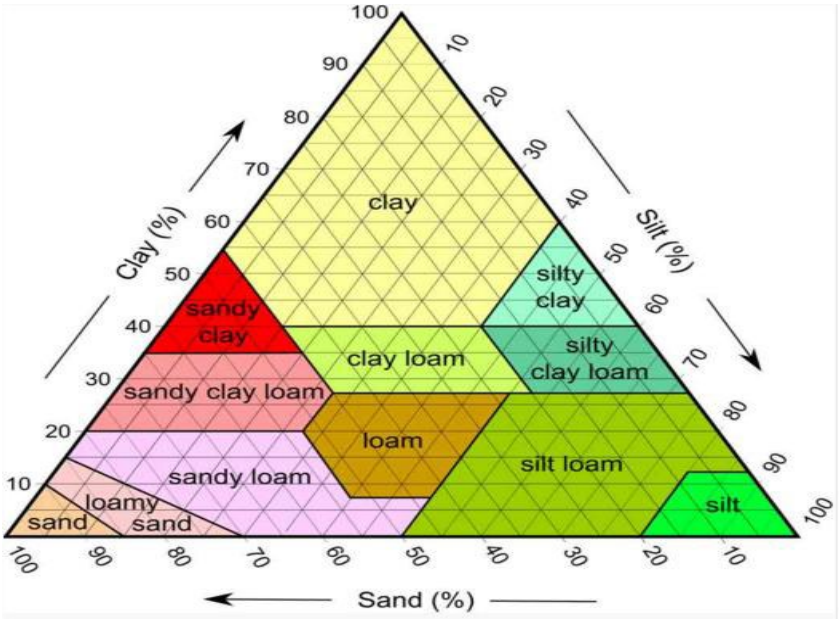



Figure 6-2 Classification of soil texture. Mangala et al. (2016)

Table 6-3 Infiltration rate for various soil types

| | Grassland | Cultivated land |
|---|---|---|
| Soil type | mm/hour | mm/hour |
| Clay | 6.5 | 2.5 |
| Silt loam | 9 | 4 |
| Clay loam | 7.5 | 5 |
| Loam | 9 | 5 |
| Fine sandy loam | 10 | 6.5 |
| Sandy loam | 11.5 | 6.5 |
| Loamy sand | 16.5 | 9 |
| Sandy loam | 19 | 10 |

Mangala et al. (2016).

**Plant interception**

The interception of an applied pesticide by the target crop is depended on the growth-phase of a crop, as this determines what fraction of the applied substance remains on the leaves and stems of the plant and what fraction reaches the soil surface. The interception fraction by various crops ranges from 0% to approximately 90%. For examples, the interception fractions of maize derived from field trials ranges between 20% and 90% depending on the growth phase (Linders et al., 2000. During the leaf development phase the interception fraction is small compared to during the ripening phase. This means, more pesticides are available for runoff during the early development phase of the crop than ripening phase because of varying interception fractions owing to these phases.

## 6.5. Parameters in higher tier runoff models

### The Pesticide Root Zone Model (PRZM)

The Pesticide Root Zone Model (PRZM) (Carsel et al., 1985) is widely used by a number of regulatory authorities (e.g. United States, Canada, European Union, Australia) and has been regularly updated over time (currently in its fifth version). PRZM5 is a process model that estimates what happens to a pesticide in a farmer's field on a day-to-day basis (Young and Fry, 2016). It considers factors such as rainfall and evapotranspiration as well as how and when the pesticide is applied. It has two major components: hydrology and chemical transport.

The hydrologic component for calculating runoff and erosion of soil is based on the Soil Conservation Service (SCS) curve number technique and the Universal Soil Loss Equation (USLE) (NRCS, 2003; Wischmeier and Smith, 1978). This approach is widely used in a number of other hydrological models, including the Soil Water Assessment Tool (SWAT – Neitsch et al., 2005) and the ACRU model developed in South Africa (Schulze, 1989).

Evapotranspiration of water is estimated from pan evaporation data. Total evapotranspiration of water includes evaporation from crop interception, evaporation from soil, and transpiration by the crop. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point, and curve number.

The chemical transport component simulates pesticide application on the soil or on the plant foliage. Dissolved, sorbed, and vapor-phase concentrations in the soil are estimated by considering surface runoff, erosion, degradation, volatilization, foliar washoff, advection, dispersion, retardation, among others.

PRZM5 caters for the input of environmental exposure scenarios that represent a unique combination of climatic conditions, crop specific management practices, soil specific properties, site specific hydrology, and pesticide specific application and dissipation processes. Each simulation is conducted using multiple years of rainfall data to cover year-to-year variability in runoff. Daily edge-of-field loadings of pesticides dissolved in runoff waters and sorbed to sediment, as predicted by PRZM5, are discharged into a water body (the parameters and dimensions of which can be specified) simulated by the Variable Volume Water Model (VVWM).

Data requirements for PRZM5 are summarised in Table 6-4 and include weather, soil, field management, cropping and physicochemical data. Relevant sources of data for applying the model in South Africa are also provided in Table 6-4. In summary all data required as input into the PRZM5 model is available in South Africa, the sources of which are discussed in more detail in the sections below.

Table 6-4 Data requirements and sources of data for running the PRZM5 model in South Africa.

| Date Type | Data Requirement | Data Source |
|---|---|---|
| Weather Data | Daily Rainfall | ARC/SAPWAT/WeatherSA |
| | Daily Humidity | ARC/SAPWAT/WeatherSA |
| | Daily T | ARC/SAPWAT/WeatherSA |
| | Daily T Variation | ARC/SAPWAT/WeatherSA |
| | Average Storm Duration | ARC/SAPWAT/WeatherSA |
| | Daily Solar Radiation | ARC/SAPWAT/WeatherSA |
| | Daily Pan Evaporation | ARC/SAPWAT/WeatherSA |
| | Daily Wind Speed | ARC/SAPWAT/WeatherSA |
| Soil Data | Soil Type | ARC/WR90 |
| | Core Depth | ARC/WR90 |
| | Bulk Density | SA Atlas of Climatology and Agrohydrology |
| | Soil Texture | ARC/WR90 |
| | Field Capacity | SA Atlas of Climatology and Agrohydrology |
| | Wilting Point | SA Atlas of Climatology and Agrohydrology |
| | Organic Carbon | ARC |
| Field Management Data | Field Slope | DEM |
| | Soil Erodibility | ARC |
| | Cropping Practice Factor | ACRU Manual |
| | Runoff Curve Numbers | ACRU Manual |
| | Cover Management Factors | ACRU Manual |
| Cropping Data | Emergence Date | SAPWAT 3 |
| | Maturation Date | SAPWAT 3 |
| | Harvest Date | SAPWAT 3 |
| | Max. Interception Rate (Water) | |
| | Max. Interception Rate (Pesticide) | Linders et al. (2000) |
| | Canopy Coverage | SAPWAT 3 |
| | Rooting Depth | ACRU Manual |

## 6.6. Data availability

### Weather data

*Data requirements for running PRZM model in South Africa*

Daily Rainfall: Daily rainfall is considered as the 24-hour accumulated amount of rain from 8:00 AM on any given day until 8:00 AM the following day. In addition, monthly rainfall is obtained by summing over the individual daily rainfall events.

Daily Humidity: Humidity is the amount of moisture in the air as a percentage of the amount the air can actually hold (Bureau of Meteorology, 2017). Warmer air can hold more moisture than cooler air, which means that for a given amount of atmospheric moisture, RH will be lower if air is warm than it would be if the air is cool. This can be seen by comparing the daily 9am maps (higher Humidity values) with the daily 3pm maps (lower Humidity values) for any month of the year.

Daily Temperature: The mean daily temperature is the average temperature in each 24 hour period, measured at 1.5 metres above the ground level (UK Climate Projects, 2017).

Average Solar Radiation: It is referred to as solar insolation which a particular area would receive if the sun is shining at its maximum value for a certain number of hours (PV Education.Org, 2017). The average daily solar insolation in units of $kWh/m^2$ per day is sometimes referred to as peak sun hours.

Average Storm Duration: It is the period of time between the onset and end of the precipitation.
Average Pan Evaporation

Evaporation: Evaporation has historically been measured at over 750 stations in South Africa using the standard USWB Class A evaporation pan (Schulze and Maharai, 2017). This pan is supported on a low wooden frame, has a diameter of 1.2 m, a depth of 254 mm and is filled with water to 203 mm. Daily evaporation is obtained by recording the change in water level from the previous day after allowance has been made for precipitation. The A-pan maybe screened by a wire mesh to prevent birds and animals from drinking out of the pan.

Daily Wind Speed: Wind speed is caused by air moving from high pressure to low pressure usually due to changes in temperature. Each station uses an anemometer to measure wind speed at a height of approximately 1.5 meters above the surface. Every five minutes, the datalogger averages two-second pulse counts to derive 5-minute average wind speed in meters per second (m/s) (NOAA, 2017).

**Soil data**

The WR2012 is a successor for WR2005 and the intention is to provide all the data, information, GIS maps, water resource models, spreadsheets and tools to allow water resource practitioners to investigate, analyse and plan their water resources studies (www.waterresources2012.co.za). This is all available by means of a menu system same as in the WR2005 DVD. The menu system consists of the following: GIS maps, VRSM2000 (Pitman) rainfall-runoff model, WR2005 database, Reports, quaternary data spreadsheets, point rainfall, naturalised streamflow, land/water use, etc. To access the data online, short registration is required.

Soil Type: It refers to the different sizes of mineral particles in a particular soil sample. Soil is made up in part of finely ground rock particles, grouped according to size as sand and silt in addition to clay, organic material such as decomposed plant matter.

Core depth: Sampling depth for most soils is typically the tillage depth in six-inch intervals. It is vital to collect soil samples from appropriate depths because a core taken deeper or shallower may generate inconsistent results.

Bulk Density: Bulk density is an indicator of soil compaction. It is calculated as the dry weight of soil divided by its volume. This volume includes the volume of soil particles and the volume of pores among soil particles. Bulk density is typically expressed in $g/cm^3$ (Soil Quality for Environmental health, 2017).

Soil Texture: Soil texture refers to the weight proportion (relative proportion by weight percentage of sand, silt, and clay) of the mineral soil separates for particles less than two millimetres (mm) as determined from a laboratory particle-size distribution.

Field Capacity: Field Capacity is the amount of soil moisture or water content held in the soil after excess water has drained away and the rate of downward movement has decreased. This usually takes place 2-3 days after rain or irrigation in pervious soils of uniform structure and texture.

Wilting Point: It is defined as the minimal point of soil moisture the plant requires not to wilt. If moisture decreases to this or any lower point a plant wilts and can no longer recover its turgidity when placed in a saturated atmosphere for 12 hours.

Organic Carbon: Organic carbon enters the soil through the decomposition of plant and animal residues, root exudates, living and dead microorganisms, and soil biota.

**Field Management Data**

DEM: It is a digital model or 3D representation of a terrain's surface. Stellenbosch University Digital Elevation Model (SUDEM) 2016 edition gives short overview of the techniques used for generating the SUDEM and provides details of the latest version (15.15) that was released in March 2015 (Van Niekerk, 2016). It is important to understand the differences in elevation models that form part of the SUDEM. A digital elevation model is a raster-based data structure that stores elevation values which can represent the land surface without the heights of land cover (i.e. digital terrain model) or it can represent terrain and land cover height (digital surface model).

Field Slope: It is a surface of which one end or side is at a higher level than another.

Soil erodibility: It is a measure of the susceptibility of soil particles to detachment and transport by rainfall and runoff.

Cropping Practice Factor: This practice include crop production practices such as monoculture and multiple cropping.

Runoff Curve: The hydrological soil properties which in combination with the crop type are used to determine the SCS curve number used for calculating runoff.

**Other sources**

Linders et al. (2000) published data for growth specific interception of applied pesticides by various target crops. Though this data is unavailable in South Africa, but interception data for crops such as maize, potatoes, onions, peas, etc. can be used.

## 6.7. Scenarios for exposure assessment

The scenarios for exposure assessments should provide a reasonable representation of the conditions across the country, while also limiting the number of scenarios to a practical number. Since the impacts of agricultural chemicals on surface water resources are expressed in catchment areas, water management areas was a key consideration for the identification of scenarios. The 2nd Edition of the National Water Resources Strategy (DWA, 2013) lists nine water management areas, but these prove a too course delineation to adequately represent conditions across the country. The First Edition of the strategy (DWF, 2004) identified 19 areas (Figure 6-3), which provides a more representative coverage of climatic and physical conditions. The addition of one site (at Douglas) provides a more representative coverage of the Upper and Lower Orange Basins. The proposed list of 20 Scenarios (represented by towns) is provided in Table 6-5. For all scenarios, 2 soil layers are specified. The characteristics for layer one for each scenario, in relation to the Pesticide in Water Calculator (PWC; Young, 2016) are provided in Table 6-6, whereas the characteristics for layer two for each scenario are provided in Table 6-6. The abbreviations are as follows:

| | |
|---|---|
| Thick (cm): | Thickness of the layer |
| p: | Effective porosity in the horizon |
| Max cap: | Maximum field capacity in the horizon |
| Min cap: | Minimum field capacity in the horizon |
| OC%: | Organic carbon in the horizon |
| N: | Manning's N value |
| Sand%: | Percentage sand |
| Clay%: | Percentage clay |

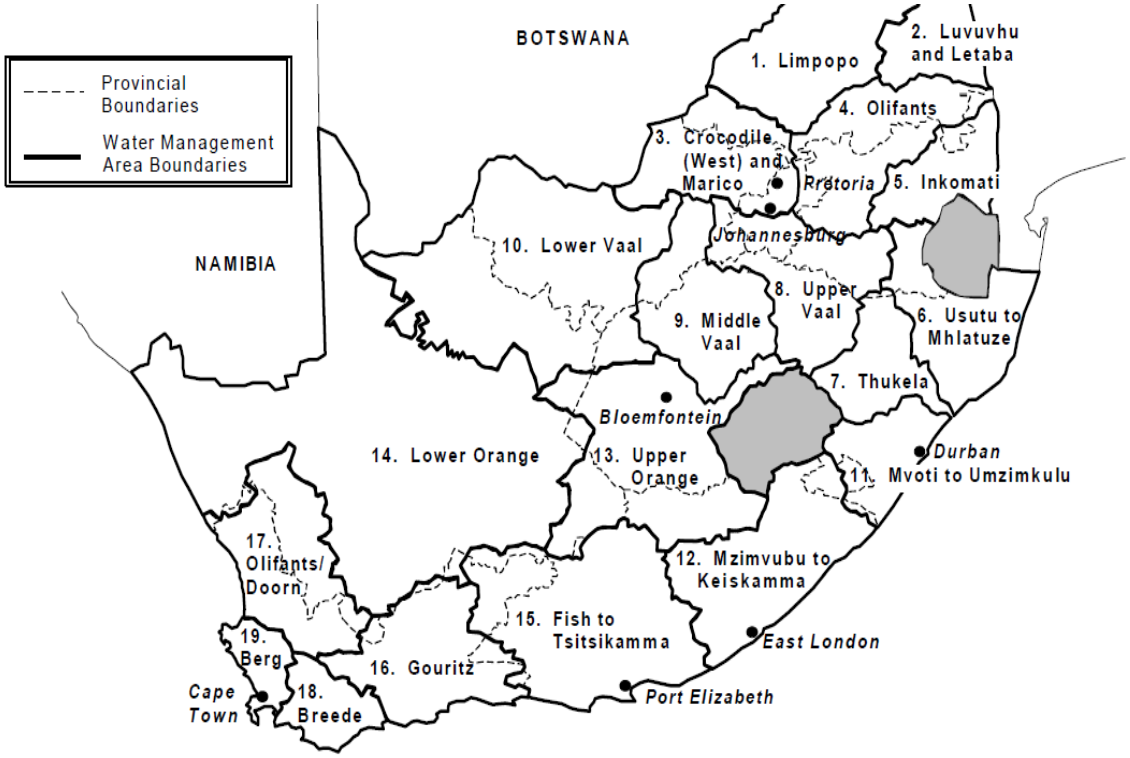



Figure 6-3 Water Management Areas from the First Edition of the Water Resources Management Strategy (DWF, 2004).

Table 6-5 Scenarios for Pesticide Exposure Assessment.

| Town | Corresponding Water Management Area (WMA) | Annual rainfall (mm)[1] |
|---|---|---|
| Malmesbury | WMA 19: Berg WMA | 490 |
| Clanwilliam | WMA 17: Olifants-Dorings WMA | 224 |
| Upington | WMA 14: Lower Orange WMA | 180 |
| Vryburg | WMA 10: Lower Vaal WMA | 477 |
| Caledon | WMA 18: Breede WMA | 596 |
| Groblersdal | WMA 4: Olifants WMA | 600 |
| Lephalale | WMA 1: Limpopo WMA | 437 |
| Welkom | WMA 9: Middle Vaal WMA | 557 |
| Brits | WMA 3: Crocodile (West) and Marico WMA | 620 |
| Giyani | WMA 2: Levhuvhu & Letaba WMA | 600 |
| Nelspruit | WMA 5: Inkomati WMA | 796 |
| Standerton | WMA 8: Upper Vaal WMA | 663 |
| Dundee | WMA 7: Thukela WMA | 765 |
| Mtubatuba | WMA 6: Usutu to Mhlatuze WMA | 967 |
| Mthatha | WMA 12: Mzimvubu to Keiskamma WMA | 693 |
| Pietermaritzburg | WMA 11: Mvoti to Mzimkulu WMA | 897 |
| Graaff-Reinet | WMA 15: Fish to Tsistsikamma WMA | 315 |
| Oudtshoorn | WMA 16: Gouritz WMA | 332 [2] |
| Douglas | WMA 14: Lower Orange WMA | 334 |
| Bloemfontein | WMA 13: Upper Orange WMA | 548 |

[1]https://en.climate-data.org/ [2]https://www.weather-atlas.com

Table 6-6 Soil characteristics for layer one for each scenarios.

| | Thick (cm) | p | Max cap | Min cap | OC% | N | Sand% | Clay% |
|---|---|---|---|---|---|---|---|---|
| Malmesbury | 30 | 1.49 | 0.212 | 0.126 | 1.22 | 2 | 73.4 | 15.6 |
| Clanwilliam | 30 | 1.47 | 0.202 | 0.117 | 1 | 2 | 68.2 | 17.3 |
| Upington | 27 | 1.43 | 0.205 | 0.118 | 0.2 | 2 | 84.5 | 7 |
| Vryburg | 24 | 1.49 | 0.24 | 0.166 | 0.4 | 2 | 70.5 | 18.2 |
| Caledon | 29 | 1.43 | 0.209 | 0.121 | 1.92 | 2 | 67 | 17.4 |
| Groblersdal | 30 | 1.42 | 0.185 | 0.092 | 1.1 | 2 | 64.7 | 1.1 |
| Lephalale | 30 | 1.39 | 0.187 | 0.092 | 0.5 | 2 | 70.9 | 17.1 |
| Welkom | 30 | 1.48 | 0.215 | 0.131 | 1 | 2 | 60.9 | 22.8 |
| Brits | 30 | 1.42 | 0.349 | 0.32 | 1.4 | 2 | 57.3 | 26.3 |
| Giyani | 30 | 1.51 | 0.219 | 0.136 | 1.1 | 2 | 61.9 | 23.3 |
| Nelspruit | 30 | 1.42 | 1.77 | 0.082 | 1.3 | 2 | 59.8 | 24.4 |
| Standerton | 20 | 1.45 | 0.328 | 0.289 | 1.3 | 2 | 58.6 | 26.6 |
| Dundee | 30 | 1.5 | 0.234 | 0.156 | 1.6 | 2 | 57.5 | 25.5 |
| Mtubatuba | 30 | 1.37 | 0.181 | 0.085 | 2.8 | 2 | 62.9 | 25.4 |
| Mthatha | 30 | 1.5 | 0.24 | 0.148 | 1.98 | 2 | 51.3 | 25.6 |
| Pietermaritzburg | 30 | 1.54 | 0.256 | 0.166 | 2.15 | 2 | 48.2 | 29.3 |
| Graaff-Reinet | 29 | 1.47 | 0.218 | 0.134 | 1.4 | 2 | 57 | 22 |
| Oudtshoorn | 28 | 1.45 | 0.206 | 0.118 | 0.8 | 0.03 | 62.4 | 22.3 |
| Douglas | 23 | 1.49 | 0.221 | 0.19 | 0.5 | 0.03 | 63.3 | 21 |
| Bloemfontein | 30 | 1.54 | 0.24 | 0.166 | 0.56 | 0.03 | 65 | 22 |

**Table 6-7:** Soil characteristics for layer two for each scenarios.

| | Thick(cm) | p | Max cap | Min cap | OC% | N | Sand% | Clay% |
|---|---|---|---|---|---|---|---|---|
| Malmesbury | 56 | 1.52 | 0.263 | 0.18 | 0.32 | 2 | 73.4 | 15.6 |
| Clanwilliam | 49 | 1.5 | 0.222 | 0.134 | 0.3 | 2 | 68.2 | 17.3 |
| Upington | 38 | 1.42 | 0.219 | 0.122 | 0.1 | 2 | 84.5 | 7 |
| Vryburg | 2 | 1.57 | 0.246 | 0.166 | 0.25 | 2 | 70.5 | 18.2 |
| Caledon | 17 | 1.46 | 0.224 | 0.135 | 0.77 | 2 | 67 | 17.4 |
| Groblersdal | 24 | 1.46 | 0.191 | 0.091 | 1.46 | 2 | 64.7 | 1.1 |
| Lephalale | 87 | 1.43 | 0.211 | 0.106 | 0.2 | 2 | 70.9 | 17.1 |
| Welkom | 75 | 1.54 | 0.272 | 0.203 | 0.9 | 2 | 60.9 | 22.8 |
| Brits | 84 | 1.39 | 0.369 | 0.329 | 0.48 | 2 | 57.3 | 26.3 |
| Giyani | 78 | 1.57 | 0.282 | 0.218 | 0.4 | 2 | 61.9 | 23.3 |
| Nelspruit | 73 | 1.47 | 1.97 | 0.096 | 0.5 | 2 | 59.8 | 24.4 |
| Standerton | 53 | 1.41 | 0.341 | 0.3 | 0.6 | 2 | 58.6 | 26.6 |
| Dundee | 80 | 1.54 | 0.29 | 0.228 | 0.6 | 2 | 57.5 | 25.5 |
| Mtubatuba | 89 | 1.42 | 0.202 | 0.094 | 1.2 | 2 | 62.9 | 25.4 |
| Mthatha | 38 | 1.57 | 0.234 | 0.142 | 0.9 | 2 | 51.3 | 25.6 |
| Pietermaritzburg | 48 | 1.54 | 0.295 | 0.203 | 0.98 | 2 | 48.2 | 29.3 |
| Graaff-Reinet | 76 | 1.54 | 0.267 | 0.196 | 0.51 | 2 | 57 | 22 |
| Oudtshoorn | 16 | 1.52 | 0.25 | 0.168 | 0.17 | 0.03 | 62.4 | 22.3 |
| Douglas | 4 | 1.57 | 0.264 | 0.192 | 0.24 | 0.03 | 63.3 | 21 |
| Bloemfontein | 47 | 1.56 | 0.305 | 0.25 | 0.23 | 0.03 | 65 | 22 |

Agronomic data of major crops grown in South Africa are summarised in Table 6-8. Model crops with shallow roots, medium roots and deep roots related to each scenario are used at a Tier I exposure model (Table 6-9).The outlined scenarios are designed to be used in Tier I exposure assessments, which are further outlined in Chapter 7.

Table 6-7 Crop parameters of major crops grown in South Africa[1]

| Crop | Planting date (month) | Crop emergence in days | Crop Maturity (days) | Harvest date | Average Rooting depth (cm) | Plant height (cm) |
|---|---|---|---|---|---|---|
| Apples & Pears | Perennial | Transplanted | 5-8 years | Mar-Nov | 25-100 | 700-1000 |
| Avocado | Perennial | Transplanted | 3-4 years | | 100 | 900-1000 |
| Banana | Perennial | Transplanted | 12 months | Jan-Nov | 100-200 | 300-500 |
| Beans | Aug-Mar | 7-10 | 55-65 | Nov-Jun | 60-100 | 40-50 |
| Beetroot | Aug-Jan | 7-10 days/Transplanted | 70-75 | Jan-May | 45-60 | 35-37 |
| Cabbage | Mar-Nov | 6-10 days/Transplanted | 70-160 | Jun-Jan | 45-60 | 20-30 |
| Carrots | Feb-Sep | 6-10 | 70-120 | May-Jan | 30-40 | 20-30 |
| Canola | Apr-Jun | 7-10 | 3 months | October | 25 | 50-80 |
| Citrus | Perennial | Transplanted | 2-3 years | Sep-Oct | 100-150 | 400-500 |
| Cucumber | Feb-Sep | 4 | 55-70 | | 45 | 30-40 |
| Lettuce | Sep-Jan | 4/Transplanted | 65-990 | | 45-60 | 30-40 |
| Macadamia | Perennial | Transplanted | 3-12 years | Feb-Aug | 100-150 | 500-800 |
| Maize | Sep-Jan | 7-14 days | 105-165 | 180-240 days | 80 | 100-250 |
| Onions | Jan-Apr | 7-14 days | 6-8 month | May-Sept | 45-60 | 40-50 |
| Peppers | Sep-Dec | 10-18 days/Transplanted | 65-95 | Nov-Jan | 70 | 30-45 |
| Potatoes | Aug/Sept/ Feb/March | 15-25 days | 70-150 | June/July Nov/Dec | 30-40 | 50-60 |
| Pumpkin | Aug-Jan | 7-14 days | 90-110 | Dec-Apr | 90 | 30-40 |
| Stone fruit | Perennial | Transplanted | | | 100 | |
| Soybeans | Oct-Dec | 5-7 days | 120-135 | Jan-Feb | 15-20 | 80-100 |
| Sugarcane | Feb-May | Transplanted | 12-16$^{th}$ months | Apr-Dec | 200-400 | 200-400 |
| Sunflower | Nov-Dec | 7-10 | 125-130 | Mar-Jun | 90-100 | 100-200 |
| Tobacco | Feb-May | Transplanted | 5-8 months | Aug-Oct | | 100-150 |
| Tomatoes | Aug-Dec | 7-10/Transplanted | | Jan-May | 80 | 100-150 |
| Wheat | Apr-Jun | 7-14 days | 150-170 | Aug-Jan | 80 | 90-120 |
| Vines | Perennial | Transplanted | | | 100 | 500 |

[1] ARC, 2013: Production guidelines for winter vegetables
ARC, 2013: Production guidelines for summer vegetables
www.daff.gov.za/dafweb3/branches/agricultural-prouction guidelines
www.starkeyers.co.za: vegetable production guide
www.hygrotech.co.za /product_range.php
Van Anwerpen, 1999: Sugarcane root growth and relationship with above-ground biomass
FOCUS 2014, Generic guidance for Tier 1 Focus Groundwater Assessment
Fan et al., 2016, Root distribution by depth for temperate agricultural crops. Field Crops Research journal home page: www.elsevier.com/locate/fcr

Table 6-8 Model crop parametersfor a hypothetical shallow, medium and deep rooted crop.

| Root depth | Emerge (day) | Emerge (month) | Mature (day) | Mature (month) | Harvest (day) | Harvest (month) | Root depth (cm) | Canopy cover (%) | Canopy height (cm) | Canopy holdup (cm) |
|---|---|---|---|---|---|---|---|---|---|---|
| Shallow | 1 | February | 1 | April | 30 | May | 45 | 70 | 30 | 0.76 |
| Medium | 1 | October | 1 | December | 30 | January | 80 | 75 | 150 | 0.1 |
| Deep | 1 | January (Perennial) | 1 | April? | 1095 | May? | 150 | 60 | 800 | 0.091 |

# 7. Risk Assessment Framework

*M Claassen M, T Nepfumbada, M van der Laan, JM Shadung*

## 7.1. Background

The US EPA introduced a framework for ecological risk assessment in the early 1990s (USEPA, 1992), which referred to an iterative process in tiers of complexity and cost. The 1998 Guidelines (USEPA, 1998a) expanded the notion by stating that data and models for risk assessment are often developed in a tiered fashion and that simple models that err on the side of conservatism may be used first, followed by more elaborate models that provide more realistic estimates. Similarly, effects data may also be collected using a tiered approach. The guidelines also note that tiered data should be evaluated in light of the decision they are intended to support; data collected for early tiers may not support more sophisticated needs.

In a workshop of the European Commission's "Concerted Action for Contaminated Land Rehabilitation Network for Environmental Technologies" (CLARINET, 2002; Faber, 2006), the following were among the common points:

- A framework should follow a tiered approach,
- Checklists are needed in the different tiers,
- A conceptual model should be part of the ERA in each tier,
- Generic values should be used in a first tier,
- Bioassays were recognized as valuable tools to be used in different tiers,

## 7.2. Purpose and general approach

The overall purpose of adopting a tiered approach for pesticide registration in the South African context is to support an efficient registration process where the risks expressed at a conservative Tier I assessment are acceptable, whereas the expression of unacceptable risks at this level will require assessments at a Tier II or Tier III to increase the confidence in the assessment. Conceptually the use of a tiered approach under conditions of uncertainty is demonstrated in Figure 7-1. The first graph represent two possible outcomes of a Tier I assessment. In curve "A", the assessment does not intersect with the unacceptable risk, in which case a decision can be made without further assessments. The second curve ("B"), however indicates the possibility of an unacceptable risk. In this case a Tier II assessment is done, whereby uncertainty can be reduced. Two possible outcomes are indicated by curves "C" and "D", which indicate the need for more detailed analysis in the case of curve "D", whereas curve "C" can be used to make a decision. Finally, at the Tier III level, the uncertainty is further reduced and two possible outcomes are shown by curves "E" and "F", with curve "E" supporting registration and curve "F" pointing to an unacceptable risk. Figure 7-1 demonstrates

the concept for the exposure assessment, but the effects assessment can also be conducted and different levels of confidence for the different tiers.

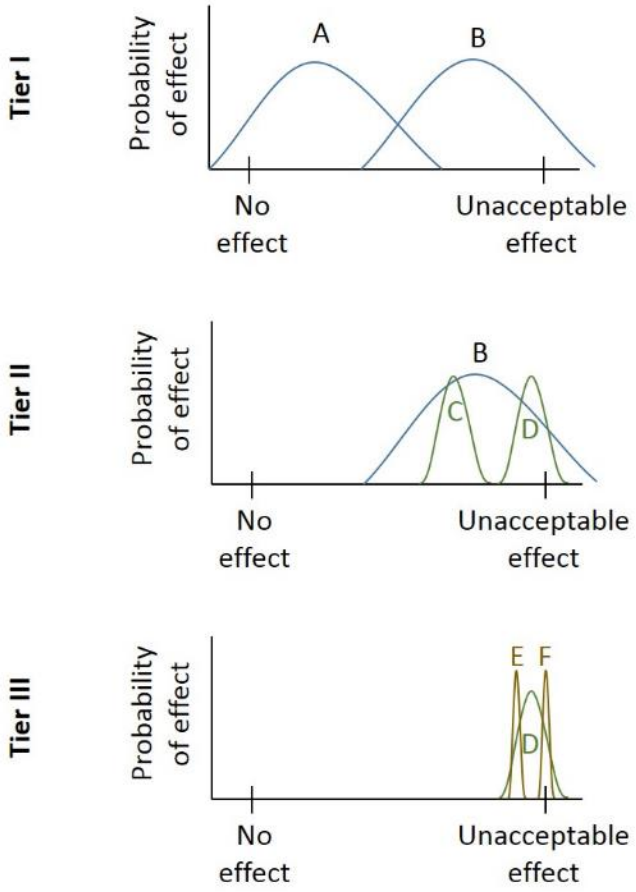



Figure 7-1 Conceptualisation of tiered approach to exposure assessment.

## 7.3. Risk assessment framework

The risk assessment framework consists of the following five components.

1) The risk assessment is conducted for different environmental scenarios.
2) For each scenario, different application rates are considered.
3) The fate and transport of the applied chemicals are then assessed.
4) The resultant exported volumes are translated into concentrations in receiving waters.
5) The concentrations are compared to effects data to determine the risk.

The five aspects with the proposed actions at each tier is presented in Table 7-1.As can be seen, the main difference between the different tiers is the differences in environmental scenarios for which the assessment is done.

Table 7-1 Tiered risk assessment for agricultural pesticides related to surface waters.

| | Tier I | Tier II | Tier III |
|---|---|---|---|
| Environmental scenarios | Use default scenarios | Adapt scenarios to be more realistic in the context of the application | Limited to detailed site-specific scenarios, but registration then only for those conditions |
| Application rates | As per the information provided by the applicant (which will become the label information) | As per the information provided by the applicant (which will become the label information) | As per the information provided by the applicant (which will become the label information) |
| Fate and transport | Use PWC[1] with default parameters | Update PWC[1] parameters according to specific scenarios | Update PWC[1] parameters according to specific conditions |
| Exposure concentrations in receiving waters | Use PWC[1] with default parameters | Update PWC[1] parameters according to specific scenarios | Update PWC[1] parameters according to specific conditions |
| Effects assessment | Use toxicity data provided by the applicant<br>- The "Peak" value predicted by PWC should not exceed the LC50[2] of target species<br>- The "4-day Average" value predicted by PWC should not be greater than the NOAEC[3] of target species | Use toxicity data provided by the applicant<br>- The "Peak" value predicted by PWC should not exceed the LC50[2] of target species<br>- The "4-day Average" value predicted by PWC should not be greater than the NOAEC[3] of target species | Use site-specific toxicity data provided by the applicant<br>- The "Peak" value predicted by PWC should not exceed the LC50[2] of target species<br>- The "4-day Average" value predicted by PWC should not be greater than the NOAEC[3] of target species |

1 - Pesticide in Water Calculator (includes the PRZM model)
2 - Concentration at which 50% of target organisms die
3 - No Observed Adverse Effect Concentration

## 7.4. Tier I Application of the Pesticide in Water Calculator

### Introduction

The Pesticide in Water Calculator (PWC) estimates pesticide concentrations in water bodies that result from pesticide applications to land. PWC is designed as a regulatory tool for users in the USEPA Office of Pesticide Programs and the Pest Management Regulatory Agency of Health Canada. PWC contains a graphical user interface shell, the Pesticide Root Zone Model (PRZM version 5.02), and the Variable Volume Water Model (VVWM version 1.02) (Young, 2016). It is based on a tool previously known as the Surface Water Concentration Calculator, but updated to simulate both surface water and ground water. In addition, the PWC has an improved volatilization routine and more batch run capabilities (USEPA, 2017; USEPA, 2019). PWC is the preferred tool for assessing the risks related to pesticide use, since it incorporates the surface water and groundwater pathways and have been used in regulatory contexts both in the USA and Canada. DAFF highlighted the constraints of using proprietary software for regulatory purposes, which also supports the use of this public access tool. It allows the regulator, the applicant and stakeholders to have equal access to the modelling platform, which will increase transparency and cooperation.

**Chemical Tab**

The chemical information required for PWC (Young, 2016) is listed in Table 7-2. It should be noted that future versions of PWC are expected to require fewer parameters (Young, pers comm.). An example of the parameters for Carbendazim is provided in Figure 7-2.

Table 7-2 Chemical information required by PWC

| Parameter | Description |
|---|---|
| Koc | The partitioning coefficient (Kd) is calculated by multiplying the sorption coefficient by the OC content of each horizon in the Crop/Land tab |
| Kd | The sorption coefficient is the Kd value entered directly into the program. All soil layers will have the same Kd with this option |
| Water Column Metabolism Half-life | Also known as the aquatic metabolism half-life. |
| Water Reference Temperature | The temperature at which the water column degradation applies. |
| Benthic Metabolism Half-life | Also known as the metabolism rate representative of the sediment |
| Benthic Reference Temperature | The temperature at which the benthic degradation applies |
| Aqueous Photolysis Half-life | The 24-hour average near-surface photolysis rate. |
| Photolysis Reference Latitude | Latitude at which the photolysis test was designed to represent. |
| Hydrolysis Half-life | The relevant hydrolysis half-life. |
| Surface Soil Half-life | The total system half-life. |
| Soil Reference Temperature | The temperature at which the soil degradation applies. |
| Foliar Degradation Half-life | The half-life of a pesticide on foliage. |
| Molecular weight | The molecular weight of the chemical. |
| Vapor Pressure | Vapor pressure of a pesticide at 25 °C. |
| Solubility (mg/L) | Solubility of the pesticide in water at 25 °C. Used indirectly to calculate the Henry's law coefficient. |
| Henry's Constant | The partitioning coefficient of a chemical between air and moist soil. |
| Air Diffusion Coefficient | The kinetic energy associated with molecular motion. |
| Heat of Henry | The enthalpy of phase change from aqueous solution to air solution. |
| Q10 | During a simulation, the degradation rate will change according to the Q10 assumption, with the entered temperature and degradation half-life as the reference point. |

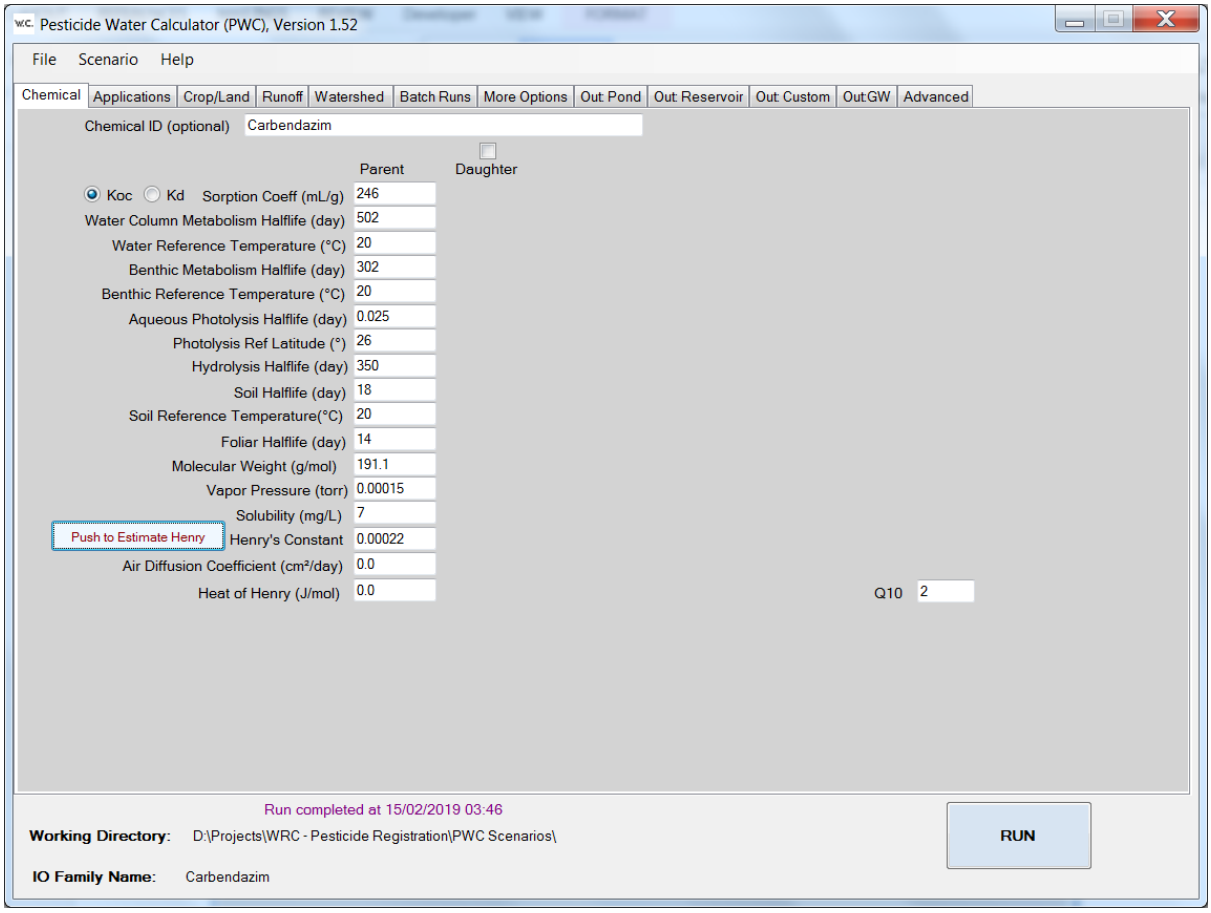



Figure 7-2 PWC with chemical parameters for Carbendazim.

### "Applications" Tab

The application information required is listed in Table 7-3, with a hypothetic example provided in Figure 7-3.

Table 7-3 Pesticide application information required by PWC

| Parameter | Description |
|---|---|
| Number of Applications/<br>Application dates/<br>Application method | Default: As per applicant information (use "maximum" specifications) |
| Days since emergence | Default: As per applicant information |
| Amount (kg/ha) | Default: As per applicant information |
| Eff (efficiency) | Default: 0.95 (Young, 2016) (as per aerial application, but used in all cases at Tier I)<br>Custom: As per application method and applicable literature |
| Drift | Default: 0. 05 (Young, 2016) (as per aerial application, but used in all cases at Tier I)<br>Custom: As per application method and applicable literature |
| "Applications occur every" | Default: 1 year<br>From year: "1"<br>to year: "last" |

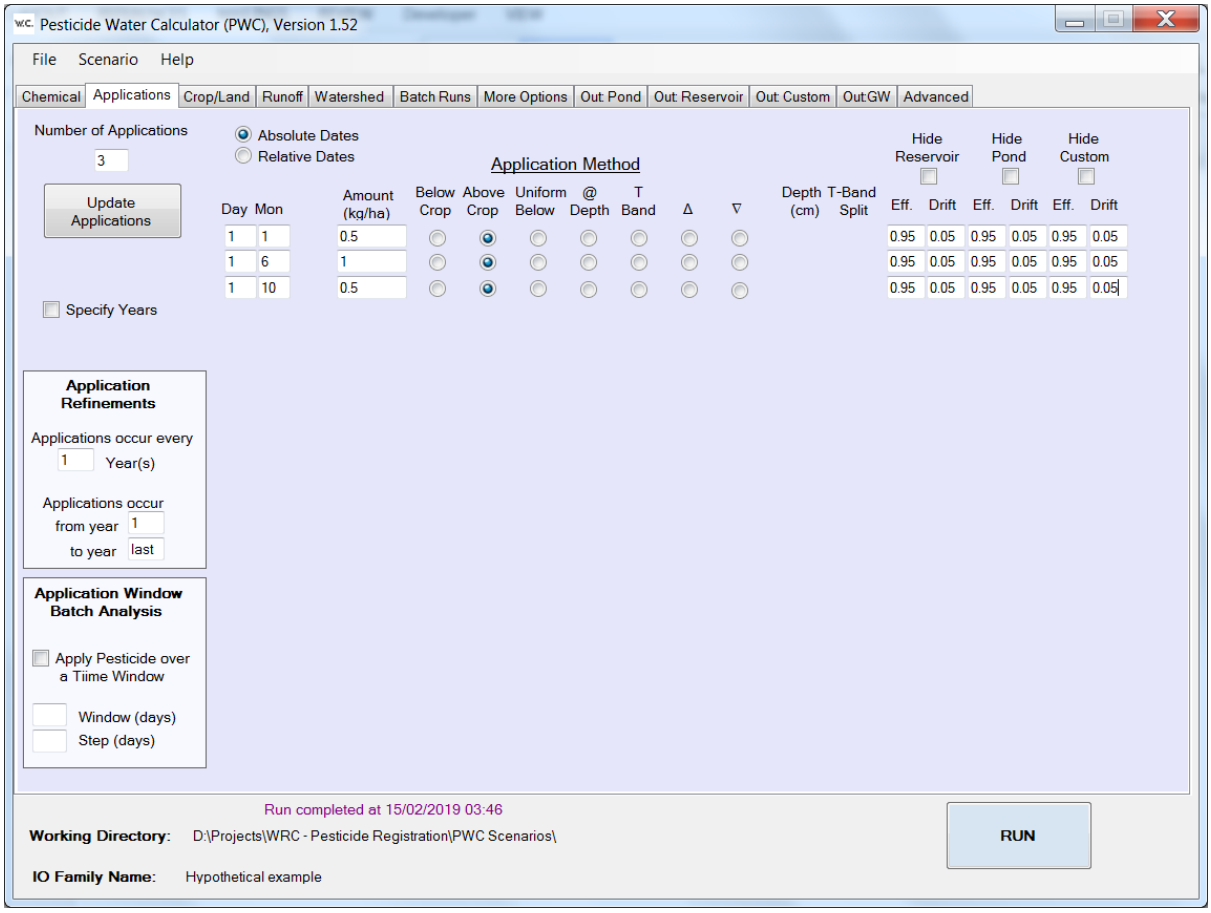


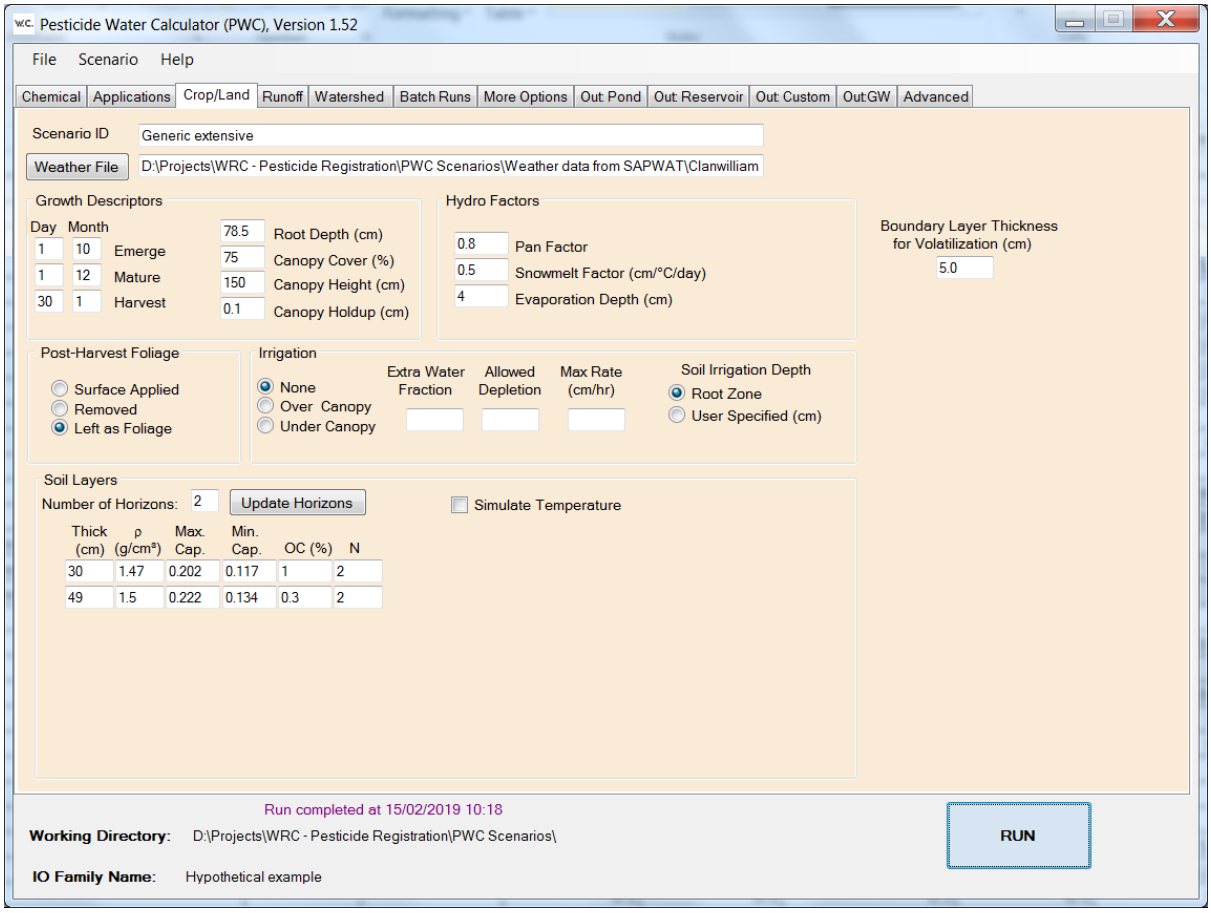

Figure 7-3 PWC “Applications” tab” with hypothetical application information.

### “Crop/Land” Tab

The scenarios outlined in Chapter 6 are used in this tab. At Tier I, the “scenario ID” is the towns in accordance with Table 6-5. The 50 year simulated weather data for each scenario, extracted from SAPWAT4 (Van Heerden and Walker, 2016), are provided with the electronic resources associated with this report. The growth descriptors for three model crops are listed in Table 6-9. For a Tier I assessment, the default values for specific parameters in this tab are (Young, 2016):

| | |
|---|---|
| Boundary Layer Thickness: | 5.0 |
| Pan factor: | 0.8 |
| Snowmelt factor: | 0.5 |
| Evaporation depth (cm): | 4.0 |
| Post-Harvest Foliage: | Left as Foliage |
| Irrigation: | None |

The “Soil Layers” information for each scenario are provided in Table 6-6 and Table 6-7. An example of the “Crop/Land” tab with a medium root depth model crop and Clanwilliam weather file and soil parameters are provided in Figure 7-4.




- *Root depth is limited to 0.5cm less than soil profile.*

Figure 7-4 PWC “Crop/Land” tab” with Clanwilliam weather and soils and a medium root depth crop.

### Runoff Tab

The runoff tab requires model parameters. For a Tier I assessment, the parameters in Table 7-4 should be used, whereas Tier II and Tier III assessments can use values that are relevant to the specific scenarios. An example of the Runoff tab for a medium rooted crop in Clanwilliam is provided in Figure 7-5.

Table 7-4 Runoff tab information required by PWC.

| Parameter | Description and default values for Tier I assessment |
|---|---|
| Day: | Default: First day of the period |
| Mon: | Default: First month of the period |
| CN: | Default for Malmesbury, Clanwilliam, Upington, Vryburg, Caledon, Groblersdal, Lephalale is 67 for shallow and medium rooted crops and 42 for deep rooted crops.<br>Defaults for Welkom, Brits, Giyani, Nelspruit, Standerton, Dundee, Mtubatuba Mthatha, Pietermaritzburg, Graaff-Reinet, Oudtshoorn, Douglas and Bloemfontein: is 85 for shallow and medium rooted crops and 79 for deep rooted crops. |
| USLE-C: | Default: 0.42 |
| N: | Default: 1 (number of chemicals in the simulation) |
| USLE K: | Default for Malmesbury, Clanwilliam, Groblersdal is 0.24<br>Default for Upington is 0.12<br>Default for Vryburg, Lephalale, Douglas and Bloemfontein: is 0.27<br>Default for Caledonis 0.22<br>Default for Welkom, Brits, Giyani, Nelspruit, Standerton, Dundee, Graaff-Reinet is 0.25<br>Default for Mtubatuba, Pietermaritzburg is 0.21<br>Default for Mthatha, Oudtshoorn is 0.23 |
| USLE LS: | Default: 1.7 |
| USLE P: | Default: 0.3 |
| IREG: | Default: 1 |
| Slope: | Default: 8% |
| PRZM5 Runoff & Erosion Extraction | Default: Use provided values (Young, 2016; p14) |
| R-Depth (cm) | Default: 2 |
| R-Decline (cm) | Default: 1.55 |
| Efficiency (Runoff) | Default: 0.226 |
| E-Depth | Default: 0.1 |
| E-Decline | Default: 0 |
| Efficiency (Eroded) | Default: 1.0 |

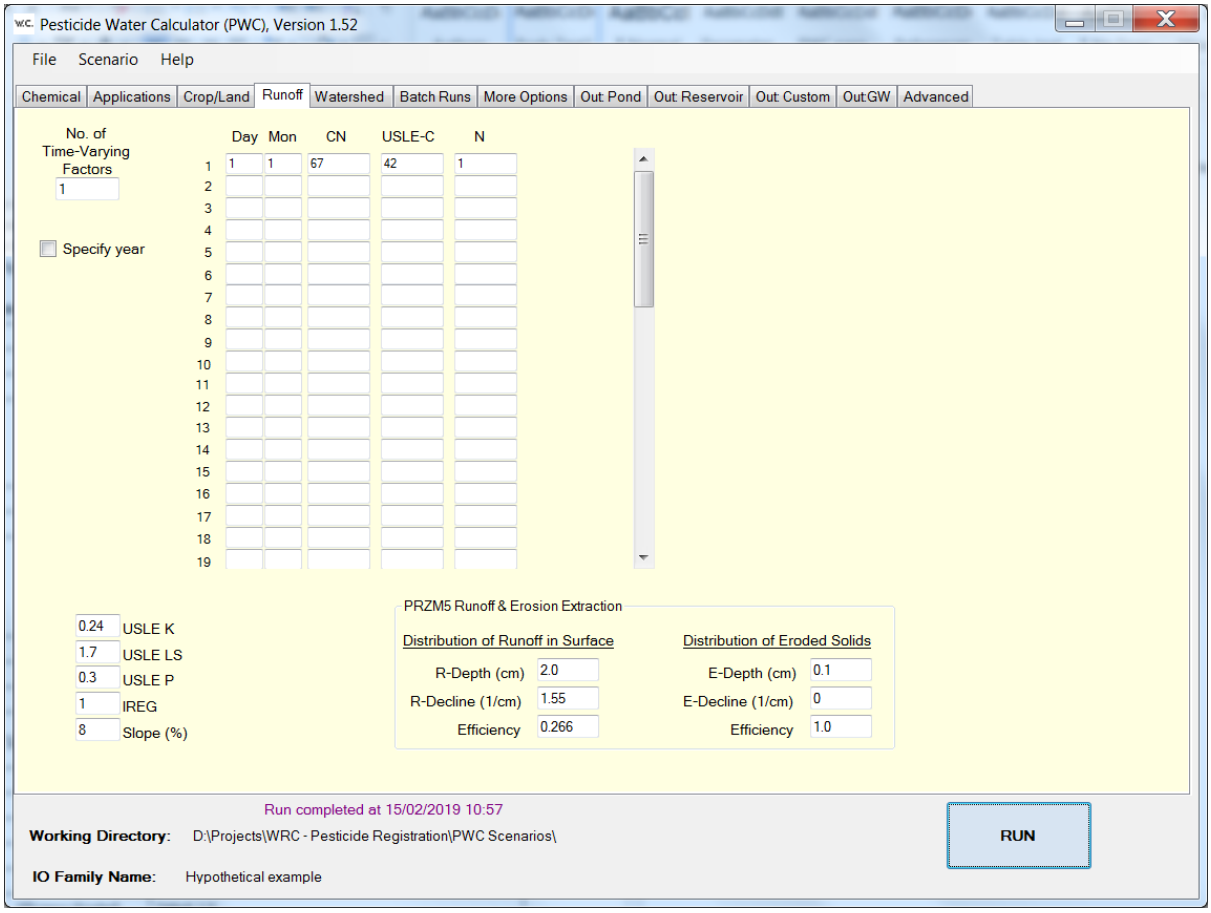



Figure 7-5 PWC “Runoff” tab” with Clanwilliam weather and soils and a medium root depth crop.

### Watershed Tab

Three scenarios are specified in the Watershed Tab. The first two are default EPA water bodies, being “EPA Pond” and “EPA Reservoir”, which are specified with constant volume and flow through. The third one is user defined, but the default for a Tier I assessment is a canal (30 cm deep and 1 m wide) that runs 50 meters from a cropped area (50% coverage) of 100 m by 1 km. This is specified as a varying volume and flow through. These and all other parameters for a Tier I assessment are as per Figure 7-6.

### Output Tabs

The result for each water body is provided in a separate tab. I typical output of the “Out: Pond” tab is provided in Figure 7-7. For the purposes of a Tier I assessment, the peak concentration under the Water Column 1-in-10 year concentration is considered the maximum concentration. Figure 7-8 provides the comparable results for the EPA Reservoir scenario, whereas the results for the user defined scenario are presented in Figure 7-9. Since the risks assessment is based on resultant surface water concentrations, the groundwater and benthic concentrations are not used in the Tier I assessment.

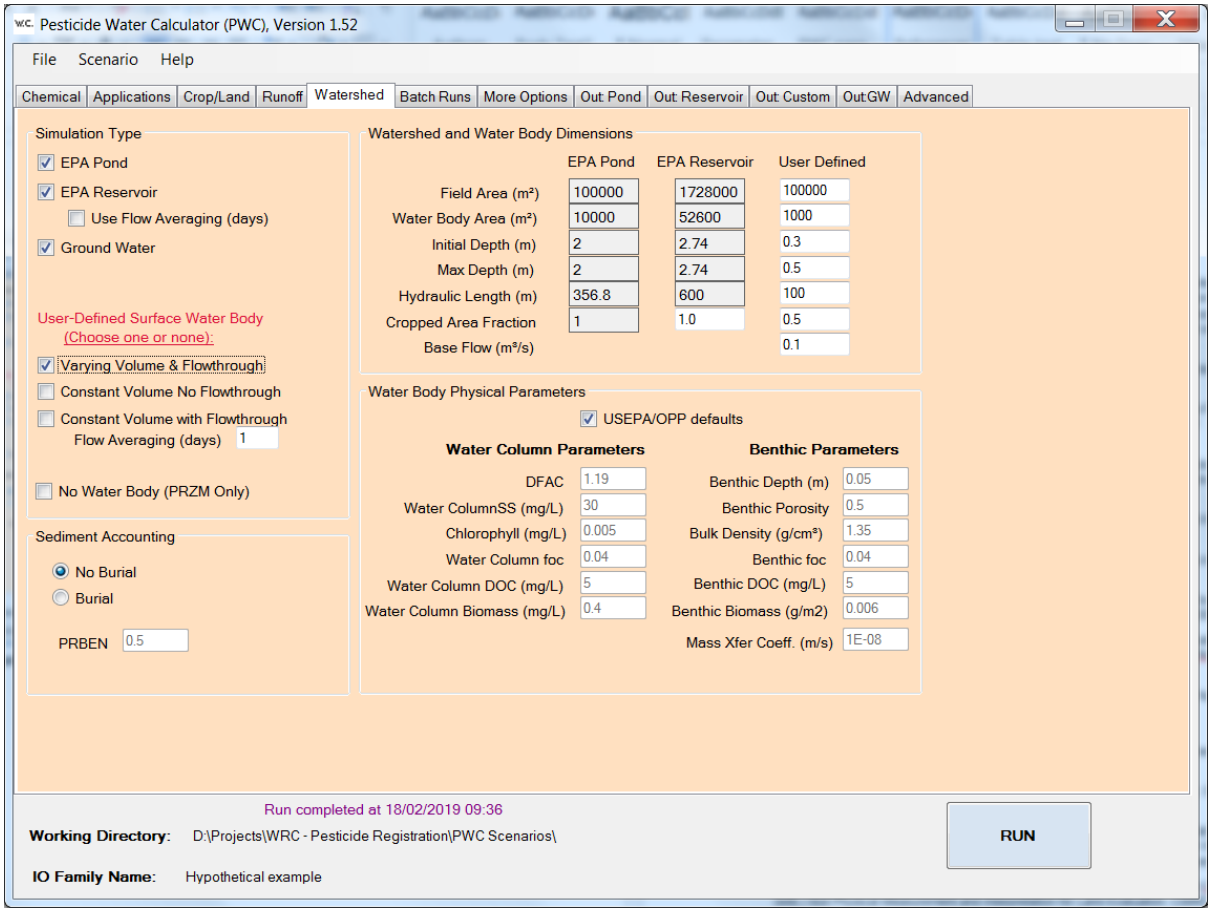



Figure 7-6 PWC “Watershed” tab parameters for water bodies.

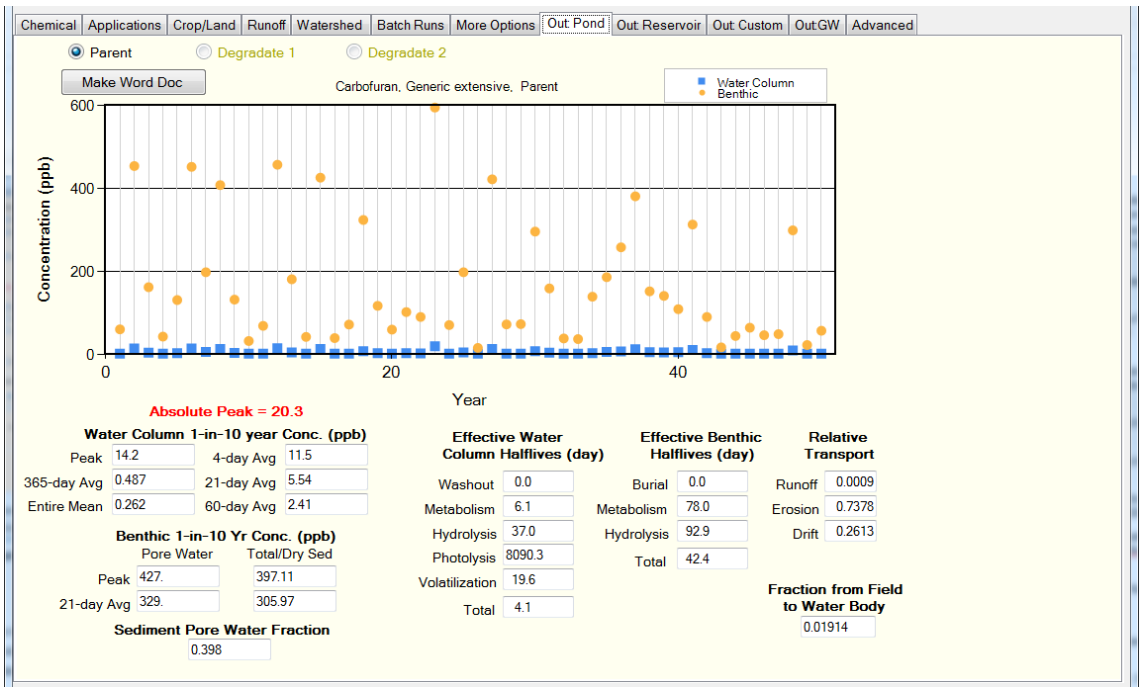



Figure 7-7 PWC “Out: Pond” tab indicating the results from the model for the EPA Pond scenario.

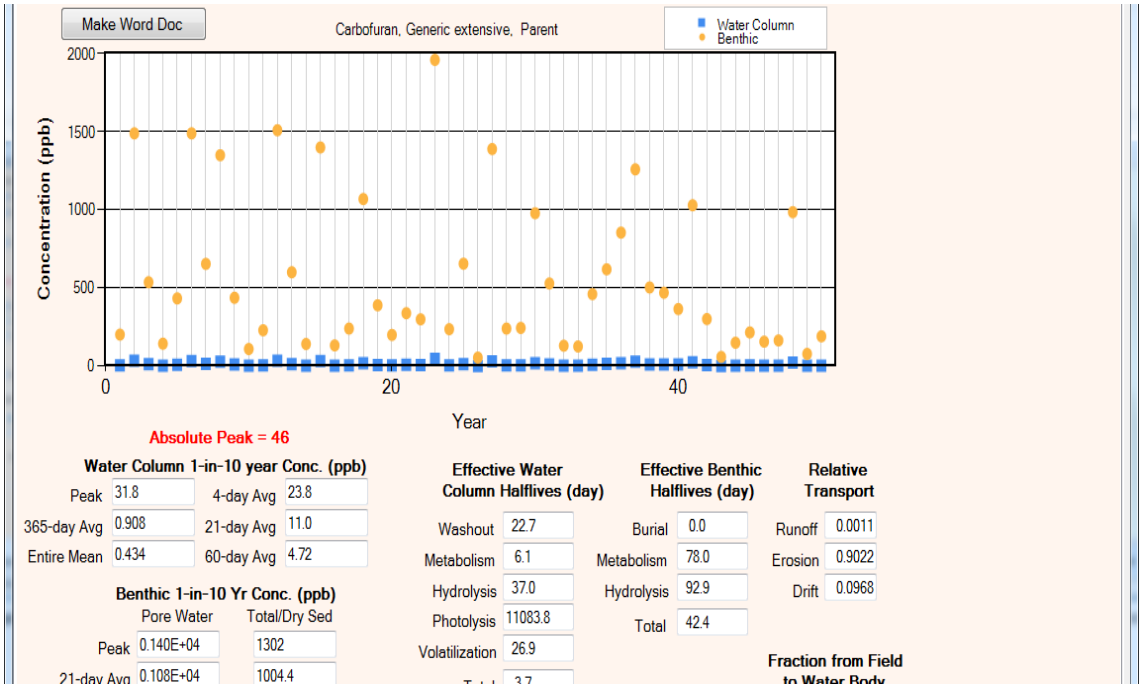



Figure 7-8 PWC “Out: Reservoir” tab indicating the results from the model for the EPA Reservoir scenario.

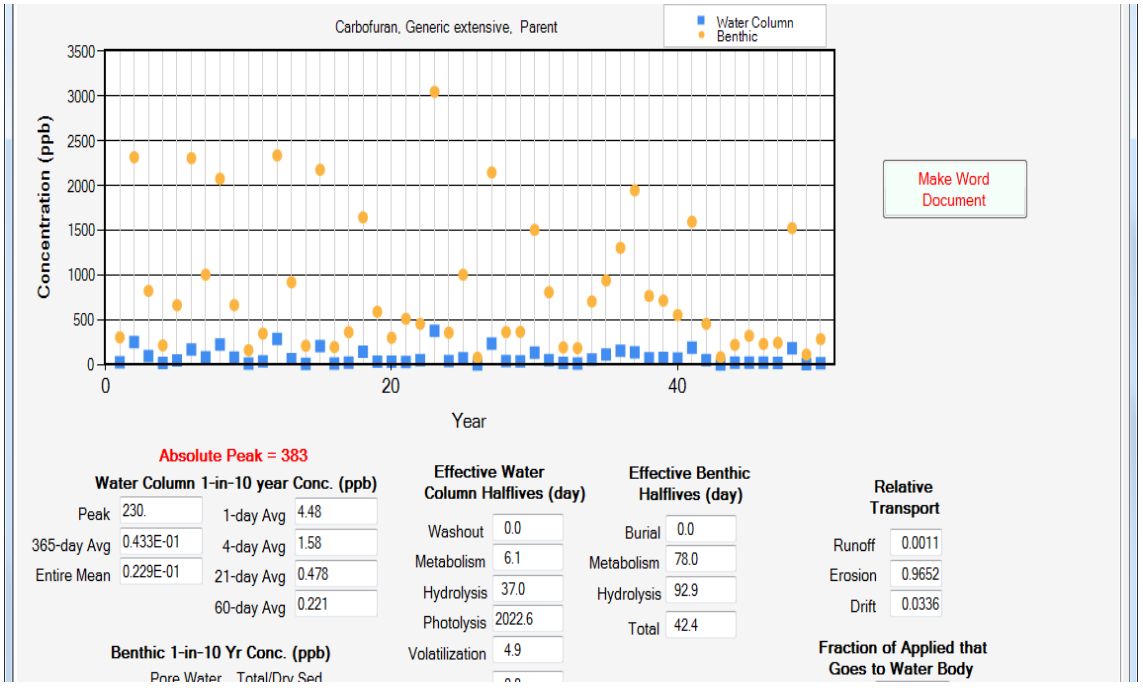



Figure 7-9 PWC “Out: Custom” tab indicating the results from the model for the user defined Tier I default scenario.

## 7.5. Field Data Compared with Pesticide in Water Calculator Results

### Purpose

The PWC model has been used in regulatory contexts in the USA and Canada and has been parameterised for South African conditions (section 7.4). To compare the model results with field data, surface and groundwater samples were taken at Komatipoort, Groblersdal, Hartswater and Ceres. Screening analysis were done on the samples for a range of agricultural and pharmaceutical compounds. Specific agricultural chemicals were selected for quantitative analysis to compare the actual field concentrations with PWC model results.

### Field samples

The study site information is summarised in Table 7-5. Due to the potential sensitive nature of some of the results, the locations are provided with a 5km accuracy. The results from the screening analyses are provided in Table 6-7, whereas the results from the definitive analyses are provided in Table 7-7. The analyses were done at LiquidTech, University of the Free State, in accordance with the method described in Odendaal et al. (2015).

Table 7-5 Field sites

| Site | Description | Approximate location |
|---|---|---|
| Komatipoort: Groundwater | Adjacent to Komati River | 25°26'9.90"S31°57'30.71"E |
| Komatipoort: Surface water | Komati River | 25°26'9.90"S31°57'30.71"E |
| Groblersdal: Groundwater | Loskop irrigation scheme | 25°10'3.27"S29°23'55.65"E |
| Groblersdal: Surface water | Olifants River | 25°10'3.27"S29°23'55.65"E |
| Hartswater: Groundwater | Near Hartswater | 27°45'11.60"S24°48'34.10"E |
| Hartswater: Surface water | Hartsriver (Pampierstad) | 27°46'50.22"S24°41'12.20"E |
| Ceres: Groundwater | Ceres | 33°22'0.20"S19°19'0.19"E |
| Ceres: Surface water | Dwars River (Ceres) | 33°22'0.20"S 19°19'0.19"E |

Table 7-6 Results from screening analysis on groundwater and surface water.

| | Komatipoort | | Groblersdal | | Hartswater | | Ceres | |
|---|---|---|---|---|---|---|---|---|
| | **Ground** | **Surface** | **Ground** | **Surface** | **Ground** | **Surface** | **Ground** | **Surface** |
| 4-deethylatrazine | X | X | X | X | | | | |
| Ametryn | | | | | | X | | |
| Amphetamine | | | | | X | X | | |
| Atenolol | | | | | | X | X | X |
| Atrazine | X | X | X | X | X | X | | |
| Atrazine-desethyl | | | | | X | X | | |
| Caffeine | | | | | | | X | |
| Carbamazepine | | | | X | X | X | X | X |
| Carbendazim | X | | | | | | | |
| Carbofuran | | | | X | | | | |
| Cetirizine | | | | | | X | | |
| Dimethenamide | | | | | | X | | |
| Diphenylhydramine | | | | | X | | | |
| Ephedrin | | | | | | X | X | |
| Fexofenadine | | | | | | | | X |
| Fluconazole | | | X | X | X | X | X | X |
| Fluroxypyr | | | | | | | X | X |
| Hexazinone | X | X | | | | | X | |
| Hordenine | | | X | | | | | |
| Imidacloprid | | | | | X | | X | X |
| Metalaxyl | | X | | | | | X | |
| Metamphetamine | | | | | | | X | X |
| Metformin | | | | | | | X | |
| Methaqualone | | | | | X | X | X | X |
| Methoxyfenozide | | | | | | | X | |
| Metolachlor | | X | X | X | X | X | X | X |
| Metribuzine | | | X | | | | | |
| Minoxidil | | | X | | | | | |
| Nicotine | | X | | | | | | X |
| Orphenadrine | | | | | | X | | |
| Phenytoin | | | | | | X | | |
| Picoxystrobin | | | | | | | | X |
| Prometryn | | | | X | | | | |
| Propazine | | | | X | | X | | |
| Propazine-2- | | | | | X | | | |
| Propiconazole | | | | | | | | X |
| Propoxur | | | X | | | | | |
| Pyrimethanil | | | | X | | | | |
| Sebuthylazine-desethyl | | X | X | X | X | | | |
| Sulfamethazine | X | X | X | X | X | X | X | X |
| Sulpiride | | | | | | X | | |
| Tebuconazole | | | | X | | | | |
| Tebuthiuron | | | | X | X | X | | |
| Terbumeton | | | | X | | | | |
| Terbutryn | | | | | | X | | |
| Terbutylazine | | X | | | X | X | | |
| Terbythylazine | | | | | | | X | X |
| Thiabendazole | | | | X | | | X | |

Table 7-7 Definitive analysis of selected agricultural chemicals

| | Site | Chemical | Concentration (ppb = ng/mL) | Limit of detection (ppb = ng/mL) |
|---|---|---|---|---|
| Ceres | Groundwater | Imidacloprid | < LOQ | 0.001 |
| | | Terbuthylazine | 0.0067 | 0.001 |
| | Surface water | Imidacloprid | 0.0075 | 0.001 |
| | | Terbuthylazine | 0.0340 | 0.001 |
| Hartswater | Groundwater | Atrazine | 0.1910 | 0.001 |
| | | Metolachlor | 0.0624 | 0.001 |
| | Surface water | Atrazine | 0.0178 | 0.001 |
| | | Imidacloprid | 0.5500 | 0.001 |
| Komatipoort | Groundwater | Atrazine | 0.0045 | 0.001 |
| | | Carbendazim | 0.0735 | 0.001 |
| | Surface water | Atrazine | 0.0463 | 0.001 |
| | | Metalaxyl | 0.0025 | 0.001 |
| Groblersdal | Groundwater | Atrazine | 0.0024 | 0.001 |
| | | Metolachlor | 0.0016 | 0.001 |
| | Surface water | Atrazine | 0.1030 | 0.001 |
| | | Metolachlor | 0.0658 | 0.001 |

**Pesticide Water Calculator modelling results**

Four modelled scenarios are presented in this section, where the Tier I input parameters for PWC are used to predict chemical concentrations in the receiving surface waters. In each case, the selected crop is deemed to be the dominant crop and the agricultural chemicals are applied according to the product label specifications.

*Ceres*

The PWC model run for Ceres is based on Imidacloprid application, at a rate of 1.5 kg/ha to apple trees (0,525 kg/ha active ingredient). The specific model parameters are provided in Figure 7-10. The model results are listed in Figure 7-11, Figure 7-12 and Figure 7-13. The model results are in line with the conservative approach for a Tier I assessment. The predicted 1-in-10 year peak values for the three scenarios were 1.31 ppb, 0.957 ppb and 0.437ppb, whereas the 60-day average values were 0.214 ppb, 0.153 ppb and 0.0202 ppb respectively. Since the actual concentrations measured in surface water was 0.075, the model produced conservative results at a Tier I assessment level.

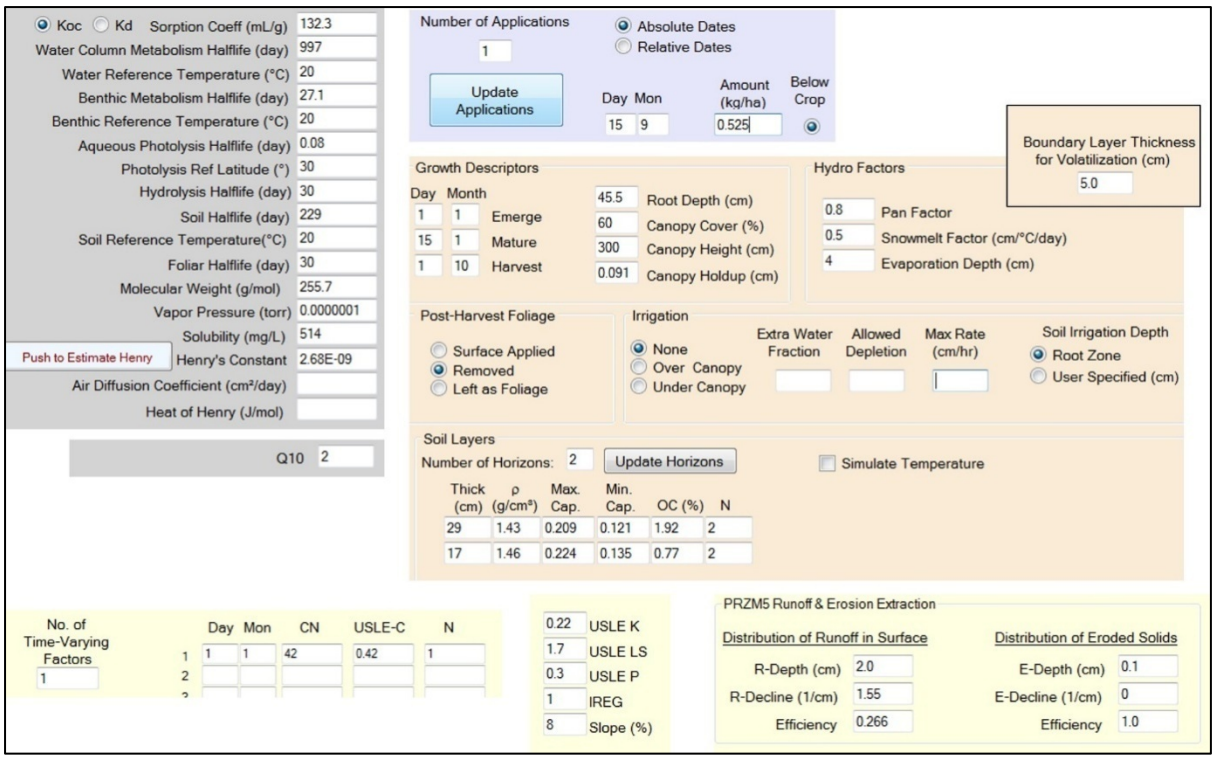



Figure 7-10 Model parameters for Imidacloprid in Ceres.

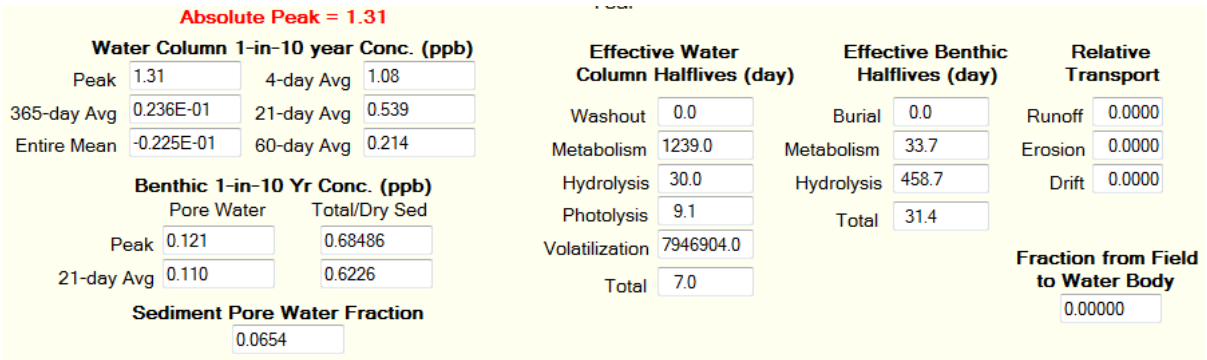



Figure 7-11 Model results for Imidaclorprid in Ceres for the EPA Pond scenario.

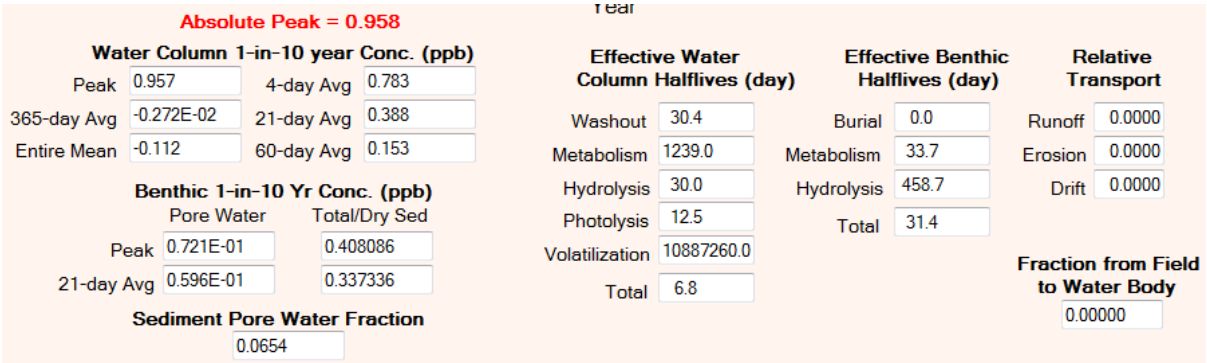



Figure 7-12 Model results for Imidaclorprid in Ceres for the EPA Reservoir scenario.

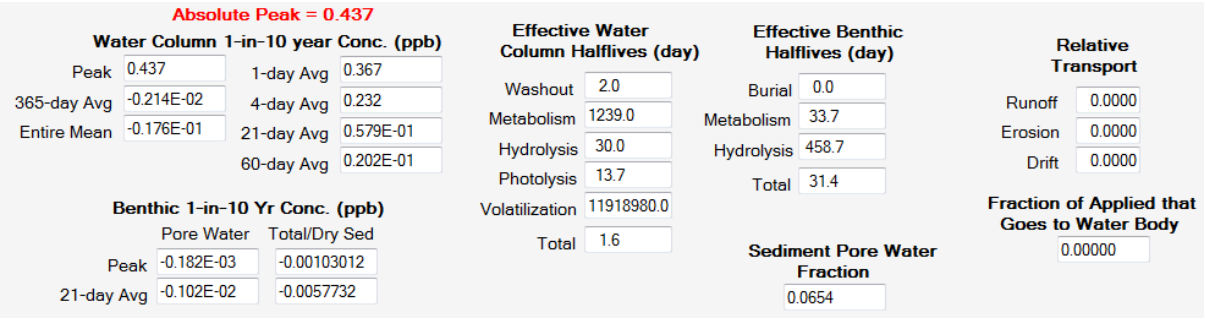



Figure 7-13 Model results for Imidaclorprid in Ceres for the Custom scenario.

*Hartswater*

The PWC model run for Hartswater is based on Atrazine applications, at a rate of 3.25 kg/ha (1.576 kg/ha active ingredient) as a pre-emergence spray and 2.5 kg/ha (1.213 kg/ha active ingredient) as a post-emergence spray to maize. The specific model parameters are provided in Figure 7-14. The model results are listed in Figure 7-15, Figure 7-16 and Figure 7-17. The model results are in line with the conservative approach for a Tier I assessment. The predicted 1-in-10 year peak values for the three scenarios were 4.06 ppb, 3.36 ppb and 2.46 ppb, whereas the 60-day average values were 0.803 ppb, 0.925 ppb and 0.129 ppb respectively. The actual concentrations measured in surface water was 0.0178, which means that the model produced conservative results at a Tier I assessment level. The PWC model met the expectations providing a conservative estimation at a Tier I assessment.

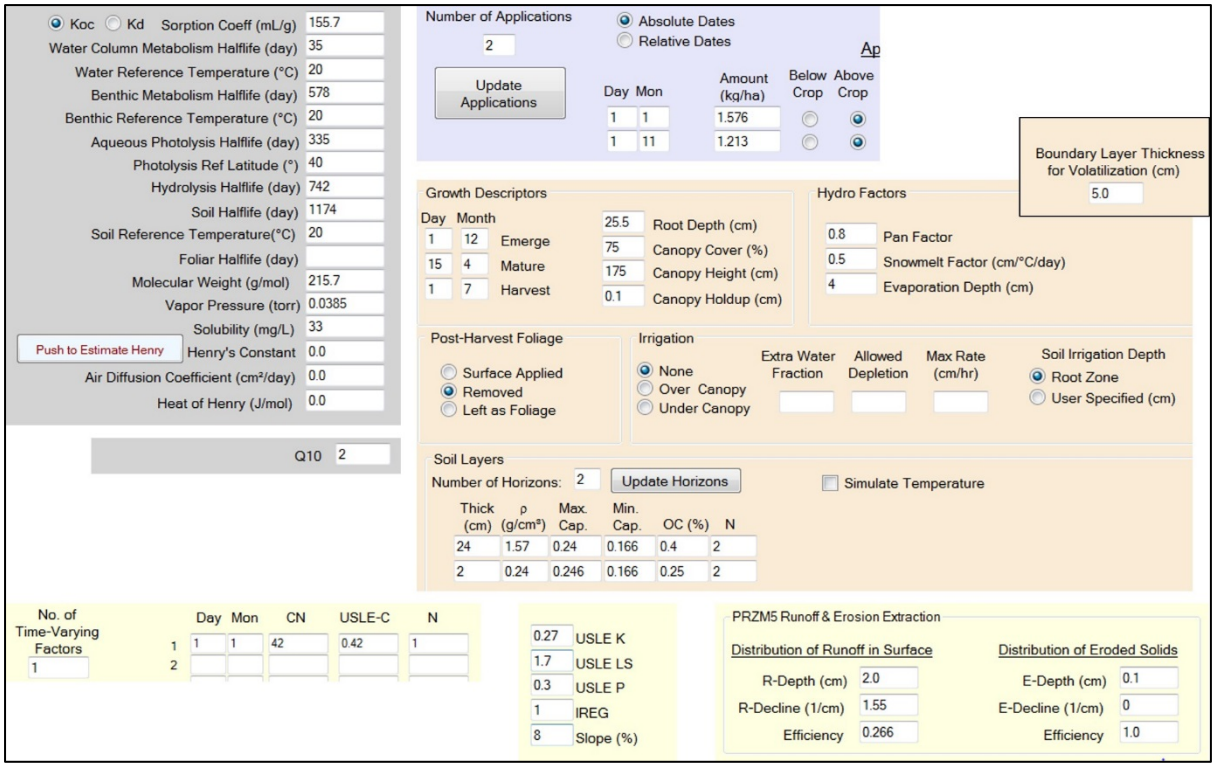



Figure 7-14 Model parameters for Atrazine in Hartswater.

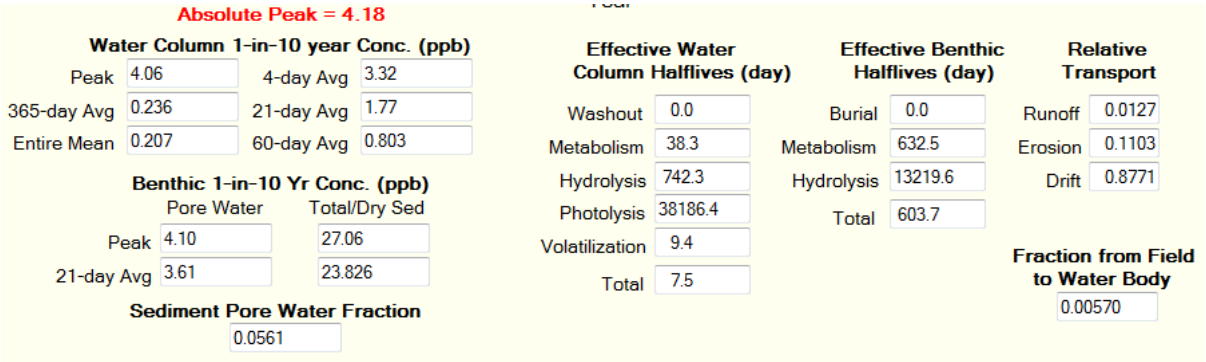



Figure 7-15 Model results for Atrazine in Hartswater for the EPA Pond scenario.

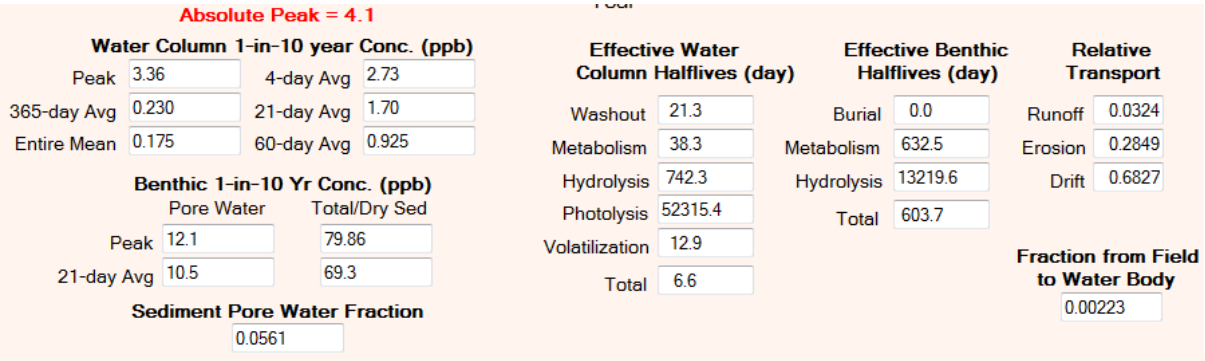



Figure 7-16 Model results for Atrazine in Hartswater for the EPA Reservoir scenario.

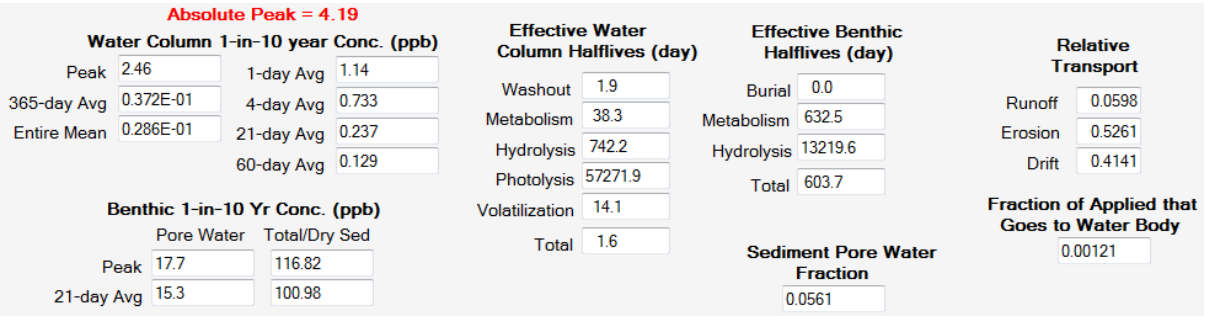



Figure 7-17 Model results for Atrazine in Hartswater for the Custom scenario.

*Komatipoort*

The PWC model run for Komatipoort is based on Metalaxyl application, at a rate of 3.15 L/ha (0.315 kg/ha active ingredient) to tomatoes, with a follow-up dosage after 10 days. The specific model parameters are provided in Figure 7-18. Note that the soil maximum capacity was reduced to 0.425, since higher values lead to "*Water capacity exceeds saturation*". The model results are listed in Figure 7-19, Figure 7-20 and Figure 7-21. The model results are in line with the conservative approach for a Tier I assessment. The predicted 1-in-10 year peak values for the three scenarios were 5.42 ppb, 6.42 ppb and 6.53 ppb, whereas the 60-day average values were 4.24 ppb, 1.92 ppb and 0.373 ppb respectively. Since the actual concentrations measured in surface water was 0.0025, the model produced conservative results at a Tier I assessment level.

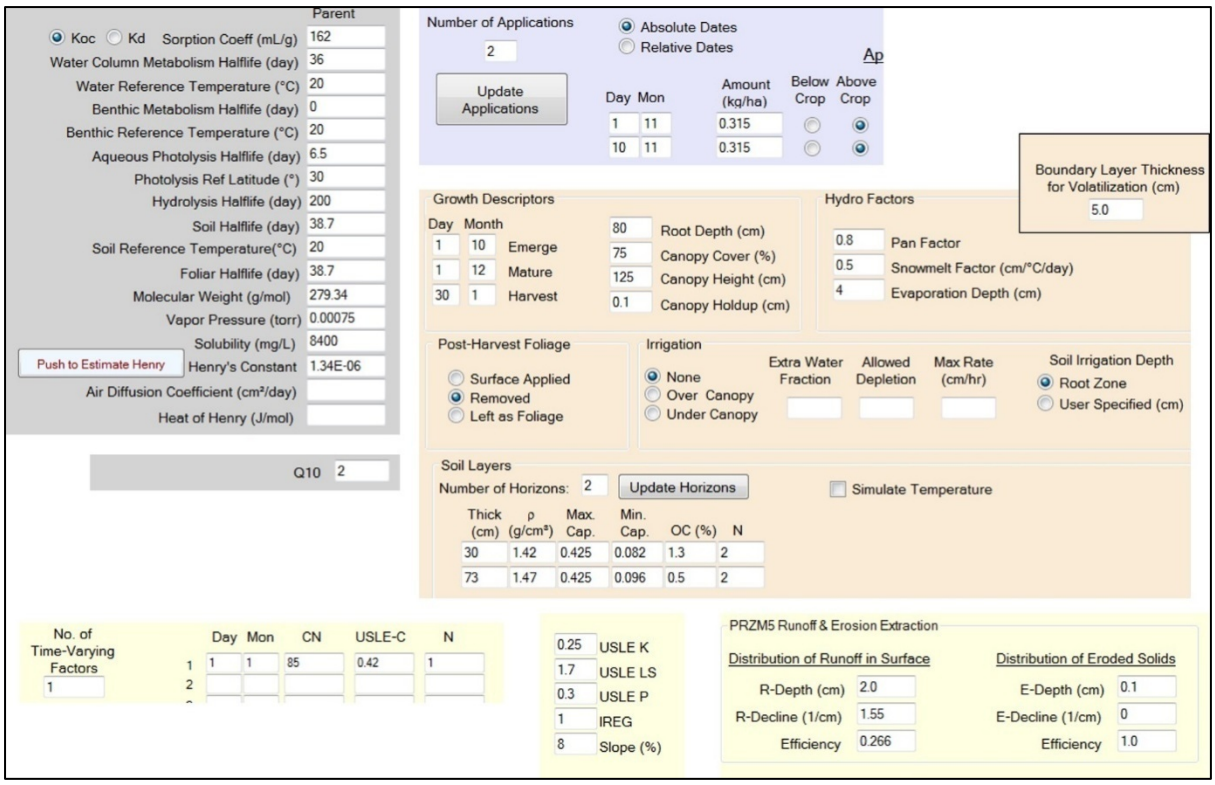



Figure 7-18 Model parameters for Metalaxyl in Komatipoort.

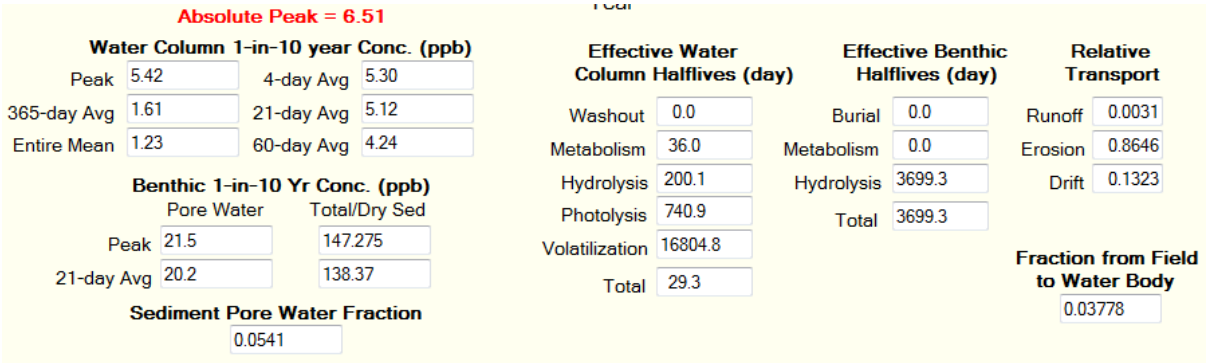



Figure 7-19 Model results for Metalaxyl in Komatipoort for the EPA Pond scenario.

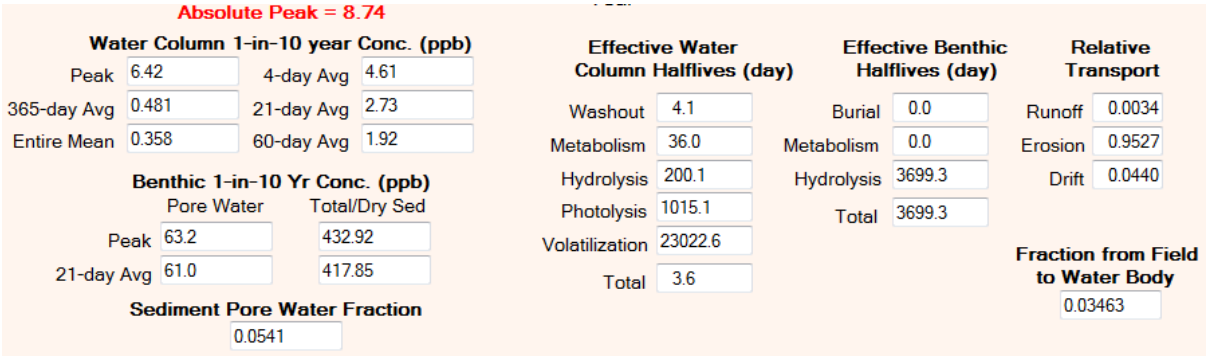



Figure 7-20 Model results for Metalaxyl in Komatipoort for the EPA Reservoir scenario.

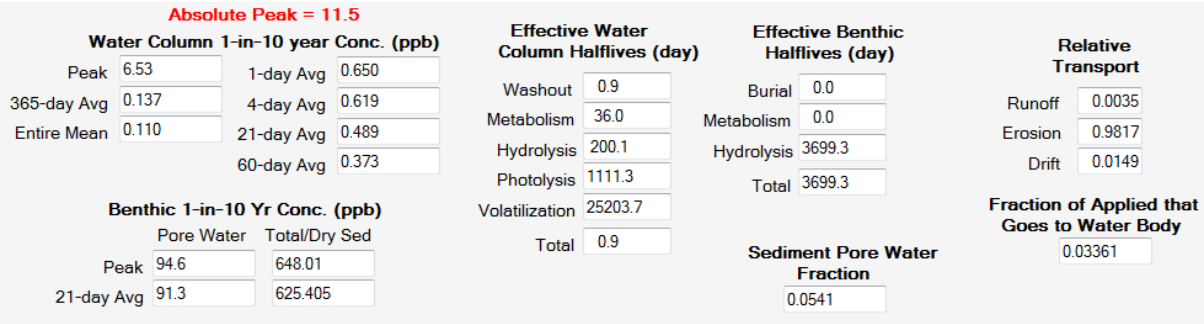



Figure 7-21 Model results for Metalaxyl in Komatipoort for the Custom scenario.

*Groblersdal*

The PWC model run for Groblersdal is based on Metolachlor pre-emergence application, at a rate of 0.5 L/ha (0.480 kg/ha active ingredient) to maize. The specific model parameters are provided in Figure 7-22. The model results are listed in Figure 7-23, Figure 7-24 and Figure 7-25. The model results are in line with the conservative approach for a Tier I assessment. The predicted 1-in-10 year peak values for the three scenarios were 1.34 ppb, 2.35 ppb and 2.25 ppb, whereas the 60-day average values were 0.444 ppb, 0.480 ppb and 0.069 ppb respectively. Since the actual concentrations measured in surface water was 0.0658, the model provided conservative estimates at the Tier I assessment level.

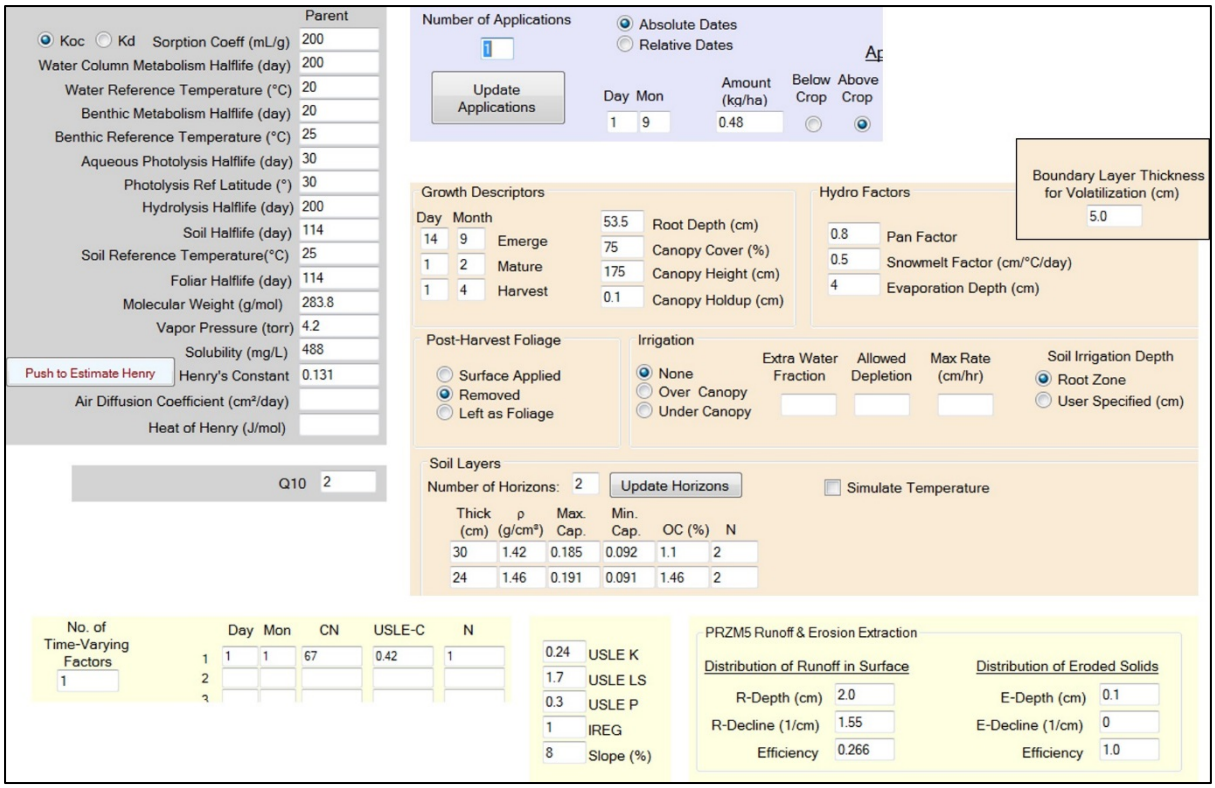



Figure 7-22 Model parameters for Metolachlor in Groblersdal.

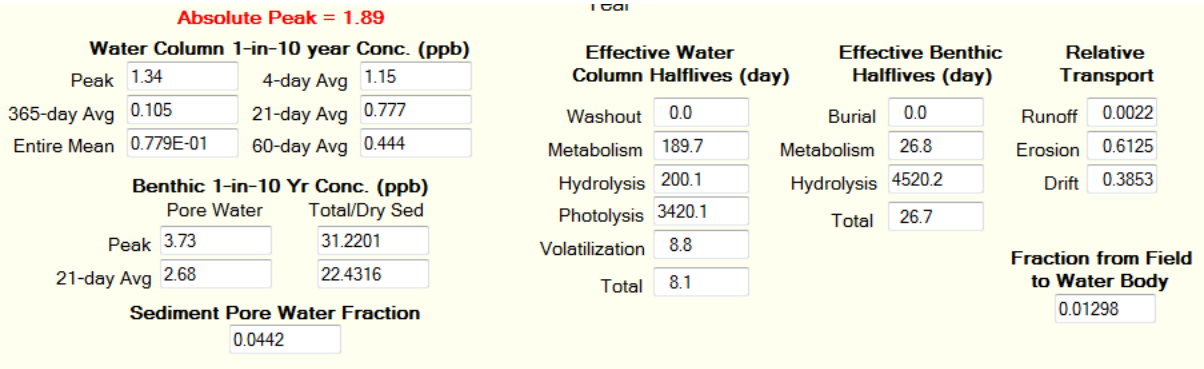



Figure 7-23 Model results for Metolachlor in Groblersdal for the EPA Pond scenario.

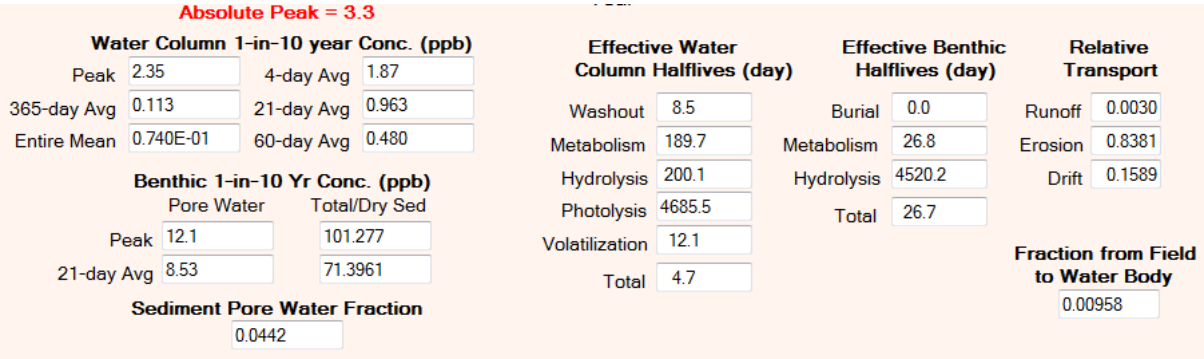



Figure 7-24 Model results for Metolachlor in Groblersdal for the EPA Reservoir scenario.

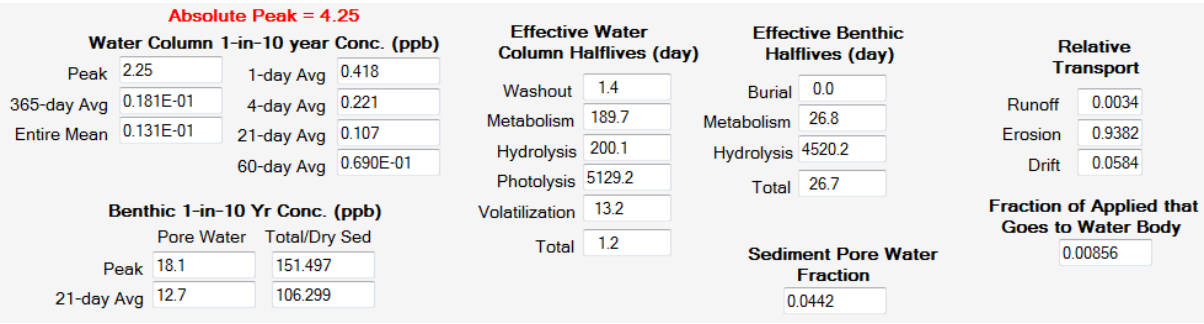



Figure 7-25 Model results for Metolachlor in Groblersdal for the Custom scenario.

### Conclusion

The above comparisons support the use of the PWC model platform for pesticide registration in South Africa. The risk assessment framework in Table 7.1 provides guidance on the application of the tools at Tier II and Tier III levels.

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