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# Dutch Environmental Indicator for plant protection products, version 2

Input, calculation and aggregation procedures

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## **Dutch Environmental Indicator for plant protection products, version 2**

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AMA van der Linden, RIVM

JG Groenwold, Alterra

R Kruijne, Alterra

R Luttik, RIVM

RCM Merkelbach, Alterra

Contact:

AMA van der Linden

Laboratory for Ecological Risk Assessment

Ton.van.der.Linden@rivm.nl

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## Abstract

### **Dutch Environmental Indicator for plant protection products, version 2**

Input, calculation and aggregation procedures

The Dutch Environmental Indicator for plant protection products (NMI) is a software package used for calculating the potential environmental impact of plant protection products, which are used in agriculture. This report gives an overview of input data and calculation and aggregation procedures used to estimate the emissions and potential impacts of these products.

Key words:

environmental impact, indicators, pesticides, sustainable plant protection



## Rapport in het kort

### **Nationale milieu-indicator voor gewasbeschermingsmiddelen, versie 2**

Input, aggregatie- en berekeningsmethoden.

De Nationale Milieu-Indicator voor gewasbeschermingsmiddelen is een softwarepakket dat wordt gebruikt voor de berekening van emissies en milieubelasting van deze middelen. Dit rapport geeft een beschrijving van benodigde invoergegevens van het softwarepakket en de concepten van de gebruikte aggregatie- en berekeningswijzen.

Trefwoorden:

bestrijdingsmiddelen, duurzame gewasbescherming, indicatoren, milieubelasting



# Contents

<b>Summary</b>	<b>9</b>	
<b>Samenvatting</b>	<b>11</b>	
<b>1</b>	<b>Introduction</b>	<b>13</b>
1.1	Overview of indicators	13
1.2	General principles	14
1.3	Running the system, input and output	15
1.4	Limitations	15
1.5	Set-up of the report	16
<b>2</b>	<b>Input data</b>	<b>17</b>
2.1	Geographical information	17
2.2	Soil data	18
2.3	Hydrological data	18
2.4	Climate data	18
2.5	Crops	18
2.6	Plant protection product use data	19
2.7	Application techniques	21
2.8	Drift	23
2.9	Substance fate and ecotox data	24
<b>3</b>	<b>Emission indicators</b>	<b>25</b>
3.1	Air	27
3.2	Groundwater	32
3.2.1	Metamodel of PEARL	33
3.3	Surface water	36
<b>4</b>	<b>Effect indicators</b>	<b>39</b>
4.1	Soil	39
4.1.1	Soil exposure concentration, single application	39
4.1.2	Soil exposure concentration, multiple applications	40
4.1.3	Potential acute effects in soil	41
4.1.4	Potential chronic effects in soil	42
4.2	Groundwater	43
4.2.1	Groundwater exposure concentration	43
4.2.2	Potential effects in groundwater	44
4.3	Surface water	44
4.3.1	Surface water acute exposure concentration, single application	44
4.3.2	Surface water acute exposure concentration, multiple applications	45
4.3.3	Potential acute effects in surface water	47
4.3.4	Potential chronic effects in surface water	48
4.4	Terrestrial organisms	48
4.4.1	Dietary exposure of birds and mammals by sprayed pesticides	49
4.4.2	Potential effects for the terrestrial ecosystem	51

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<b>References</b>	<b>55</b>
<b>Appendix 1 Glossary</b>	<b>57</b>
<b>Appendix 2 List of symbols</b>	<b>59</b>
<b>Appendix 3 Crops included in NMI version 2</b>	<b>63</b>
<b>Appendix 4 Crop interception fractions</b>	<b>65</b>
<b>Appendix 5 NMI database input for substances</b>	<b>67</b>
<b>Appendix 6 Input parameters for terrestrial ecosystem</b>	<b>69</b>

## Summary

The Dutch Environmental Indicator for plant protection products (NMI) is a software package used for calculating the potential environmental impact of plant protection products, which are used in agriculture (both arable crops and greenhouse crops). This report gives an overview of input data and calculation procedures used to estimate the emissions and potential impacts. Calculations are performed for grid cells of 100 ha each, using geographical and time dependent information; results of the calculations therefore vary in space and time.

The NMI currently is capable of calculating the following indicators:

- emission of plant protection products (PPP) to air resulting from volatilisation during application, volatilisation from the plant canopy and volatilisation from the soil; for greenhouse crops, emission to air by volatilisation from the greenhouse is calculated;
- emission of PPP to groundwater resulting from leaching, including leaching from greenhouse crops rooting in soil;
- emission of PPP to surface water resulting from lateral drainage and drift during application, including lateral drainage from greenhouse crops rooting in soil;
- emissions resulting from some point sources from greenhouses and bulb disinfections to surface water;
- potential acute and chronic effects in the soil of treated fields;
- potential acute and chronic effects in surface water resulting from drift to surface water;
- potential acute and chronic effects to terrestrial organisms feeding on treated fields;
- potential effects of leaching to groundwater regarding its potential use as source for drinking water.

The potential chronic effect modules are new in version 2. Apart from this a number of more technical changes were realised.

Emissions are calculated as amounts (kg) active ingredients emitted from treated fields; potential effects are expressed as Environmental Indicator Units. Results can be visualised on maps.

Furthermore, results can be given as numbers per, amongst others, crop, agricultural sector and the Netherlands as a whole.

Calculation concepts apply to a single application of a plant protection product at the field scale. Unfortunately, input information is not available for individual fields. Information on applications is derived from national investigations whereas data on land use are from national census data. The NMI is therefore best fit for applications at the national scale. Results might be less accurate when the NMI is used at the regional scale with the same input data. The accurateness will depend on the representativeness of national data for the region under investigation.



## Samenvatting

De Nationale Milieu-Indicator (NMI) voor bestrijdingsmiddelen is een softwarepakket dat gebruikt wordt voor de berekening van emissies en potentiële effecten van gewasbeschermingsmiddelen, welke in de Nederlandse landbouw (zowel vollegrond als glastuinbouw) worden gebruikt. Dit rapport beschrijft de benodigde invoergegevens en de concepten voor de berekening van de emissies en de potentiële effecten en de aggregatieprocedures. De berekeningen worden voor gridcellen van 100 ha uitgevoerd, gebruikmakend van locatiespecifieke en tijdsafhankelijke invoer. De resultaten zijn daarom ook variabel in ruimte en tijd.

De NMI bevat momenteel modules voor de berekening van:

- emissie van gewasbeschermingsmiddelen naar de lucht, inclusief de vervluchting uit kassen;
- emissie van gewasbeschermingsmiddelen naar het grondwater als gevolg van uitspoeling, inclusief de uitspoeling van grondgebonden kasteelten;
- emissie van gewasbeschermingsmiddelen naar oppervlaktewater als gevolg van laterale drainage en drift, inclusief de laterale drainage van grondgebonden kasteelten;
- emissie vanuit puntbronnen in de kasteelt en de afspoeling van erven bij de ontsmetting van bollen;
- potentiële acute en chronische effecten in de bodem van behandelde percelen;
- potentiële acute en chronische effecten in het oppervlaktewater als gevolg van de driftbelasting;
- potentiële acute en chronische effecten op terrestrische organismen die foerageren op behandelde percelen;
- potentiële effecten op het grondwater als bron voor de drinkwatervoorziening.

De modules voor de berekening van potentiële chronische effecten zijn nieuw in versie 2. Daarnaast werd een aantal meer technische aanpassingen doorgevoerd.

Emissies worden berekend als hoeveelheid (kg) werkzame stof; potentiële effecten als Milieu-Indicator Punten (MIP's). Resultaten van de berekeningen kunnen zichtbaar worden gemaakt op kaarten. Getalsmatige uitvoer is verder onder andere mogelijk per gewas, per sector en voor Nederland als geheel.

De concepten voor de berekeningen gaan uit van een toepassing van een gewasbeschermingsmiddel op veldschaal, maar de benodigde invoer is niet voorhanden voor die schaal. Gegevens over toepassingen zijn ontleend aan landelijke enquêtes. De toepassing van de NMI is dan ook vooral op landelijke schaal. Bij gebruik van dezelfde invoergegevens zullen resultaten minder betrouwbaar zijn als voor regio's wordt gerekend; de betrouwbaarheid hangt dan af van de representativiteit van de landelijke invoergegevens voor de betreffende regio. Om voor regio's betrouwbare uitvoer te krijgen zullen op de regio toegespitste invoergegevens moeten worden gebruikt.



# 1 Introduction

On behalf of the Netherlands Ministry of Agriculture, Nature and Food Quality (LNV) and the Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM) the research institutes ALTERRA and RIVM develop a computation system for the calculation of environmental indicators, called NMI. The computation system should be capable of calculating:

- loads of various environmental compartments with plant protection products;
- potential effects of these products in distinguished environmental compartments.

The purpose of the NMI is to support the evaluation of plant protection programmes of the Dutch Government, such as laid down in the policy document ‘Nota Duurzame Gewasbescherming (Sustainable Plant Protection)’ (LNV, 2004).

The NMI builds upon earlier Dutch studies regarding the development of environmental indicators for pesticides (Brouwer et al., 1999; Brouwer et al., 2000). In these studies, emissions of plant protection products to surface water and groundwater, potential effects on aquatic organisms and potential effects on the quality of groundwater were calculated according to methods which, at the time, were also used in pesticide registration. In addition, potential effects on birds were calculated. However, the calculation method for this differed slightly from the method used in registration. Characteristic for the calculation methods used in pesticide registration in that period was the use of a few fixed scenarios; environmental conditions were highly standardised, temporal variations were categorised into two seasons and spatial differences were not taken into account. The NMI differs from the earlier studies especially with regard to the spatial and temporal variability.

## 1.1 Overview of indicators

The NMI currently is capable of calculating the following indicators:

- emission of plant protection products (PPP) to air resulting from volatilisation during application, volatilisation from the plant canopy and volatilisation from the soil;
- emission of PPP to air by volatilisation from greenhouses;
- emission of PPP to groundwater resulting from leaching;
- emission of PPP to surface water resulting from lateral drainage and drift during application;
- emission of PPP to surface water resulting from treatment of plant material;
- potential acute effects in the soil of treated fields;
- potential chronic effects in the soil of treated fields;
- potential acute effects in surface water resulting from drift to surface water;
- potential chronic effects in surface water resulting from drift to surface water;
- potential acute effects to terrestrial organisms feeding on treated fields;
- potential chronic effects to terrestrial organisms feeding on treated fields;
- potential effects of leaching to groundwater regarding its potential use as source for drinking water;
- potential chronic effects to groundwater inhabiting organisms.

Some of the indicators require external data selection. For example, a set of reference values for ecotoxicological effects (relevant ecotoxicological concentrations) have to be chosen and this set has to be imported in the NMI database.

Modules for calculating additional indicators can and will be added to the system. The following indicators are being developed:

- potential chronic effects in surface water resulting from lateral drainage.

The set-up of the package is such that other indicators can be added quite easily.

No emissions are calculated for:

- applications of liquid soil disinfectants (the liquid soil disinfectants are not included in the national surveys on the use of PPP; for these substances the use is authorised on a case by case basis);
- non-agricultural applications (insufficiently detailed use data available; no calculation method implemented);
- surface runoff from agricultural fields (no satisfying calculation method available yet);
- seed disinfection, all methods (spraying, slurring, coating, powdering, etcetera) (no satisfying calculation method available yet; no use data for seed disinfection available);
- algae removal from the glass deck of greenhouses (no satisfying calculation method available yet);
- pheromone applications (insufficiently detailed use data; no satisfying calculation method available yet);
- rodenticide applications (bait, smoke tablets, etcetera) (no satisfying calculation method available yet).

For some of these applications the emissions are assumed to be zero due to the fact that a suitable method for their calculation has not yet been implemented or is missing; for some other applications (non-agricultural applications, seed disinfection, pheromones) sufficiently detailed information about the use of products is lacking and calculated emissions would be very uncertain.

## 1.2 General principles

All potential environmental effect indicators described in this report are based on the principle of relating predicted environmental concentrations to ecotoxicological effect concentrations or environmental concern concentrations. By definition the value of one for the ratio of the predicted environmental concentration to the ecotoxicological effect concentration is called an Environmental Indicator Unit (EIU); in Dutch: Milieu-Indicator Punt (MIP):

$$EIU = \frac{PEC}{ECC} \quad \text{Eq.1-1}$$

in which:

EIU Environmental Indicator Unit, (-)

PEC Predicted Environmental Concentration, (e.g. mg kg<sup>-1</sup> or µg dm<sup>-3</sup>)

ECC Environmental Concern Concentration, (e.g. mg kg<sup>-1</sup> or µg dm<sup>-3</sup>)

The Predicted Environmental Concentration is either an initial concentration or a long-term concentration. The initial concentration is used when assessing acute effects occurring within a few

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hours, while the long-term concentration is used when assessing chronic or semi-chronic effects due to exposure for a couple of weeks. Chapter 4 gives details of the calculation of the various indicators.

## 1.3 Running the system, input and output

The NMI is an ensemble of databases, calculation modules and report facilities. The databases contain all the information to calculate emissions and potential impacts for all registered plant protection products that are used in agriculture in the Netherlands; at this moment for the period 1998 – 2005. In order to target calculations to specific needs, the user can make selections with respect to:

- plant protection products, one – all (option to select all substances belonging to a functional group at once);
- period, month – year;
- crop, single crop – all (option to select all crops in an agricultural sector at once);
- area, municipality - whole country, (see section 1.4 for limitations);
- indicators (one – all) (several options, for example emissions only or spray applications only).

Some of the indicators require selection of (eco)toxicological endpoints before running the system. The data in the substances database need to be compatible with the selected indicator or the selected ecotoxicological endpoint (see also section 2.9 and Appendix 5). The selection of the data is not a feature of the NMI. Appropriate data have to be selected off-line and transferred to the NMI database. The user is responsible for the consistency of the data.

Output of the software package is by means of tables (output data files that can be imported in spreadsheets) and maps. The amount of output is dependent on user specifications and ranges from very huge amounts, when output for each grid cell is selected, to rather limited amounts, when only total area sums are requested.

## 1.4 Limitations

Calculations in the NMI are set up to run on the scale of one application, i.e. the field scale. The most detailed output, however, is at the scale of one square kilometre. The spatial scale at which the NMI is to be used is determined by the input data. The current database of the NMI contains input values valid for the regional scale (crop, soil and climate data) and national scale (pesticide use data). The representativeness of the use data will usually determine the reliability of the results and limit the scale at which the NMI is used. The limited experience so far has indicated that results may still be acceptable at the regional scale (Kruijne et al., 2007).

The temporal scale of the NMI is also determined by the detail of the input database. The current database contains monthly averages of input values regarding applications of plant protection products and weather data. The finest temporal resolution is therefore one month. Calculations on emissions and impacts initially are for a surface unit of 1 ha; upscaling to larger areas is based on the total treated area, i.e. results for the larger area are obtained by multiplying results for one hectare by the area on which the respective plant protection products are used.

## 1.5 Set-up of the report

Chapter 2 describes input data and parameters for the exposure and potential effect calculations, to a limited degree of detail with reference to original descriptions. Chapter 3 describes how emissions from the target areas are calculated. Finally, chapter 4 describes the calculation of Predicted Environmental concentrations and Ecological Concern Concentrations for the various environmental compartments and their organisms and the potential environmental impacts.

## 2 Input data

The NMI uses large amounts of input data, regarding:

- soil data, variable in space;
- climate data, variable in space and time (for example different long term average temperature for each month);
- crops, acreages and their distributions over the Netherlands, variable in time (two distinct years included at the moment);
- for greenhouses: the areas soil bound cultivation and substrate cultivation, variable in time;
- for greenhouses; recirculation of drainage water and recirculation of condensation water;
- PPP use data, variable in space and time, dependent on the crop;
- information on application techniques;
- crop interception data, varying with crop and growth stage;
- drift data, depending on crop, application technique and drift reduction measures;
- pesticide fate and ecotoxicology data.

The different input data are discussed in some detail in the following paragraphs.

The primary goal of the NMI is to serve as an evaluation tool. Although the NMI calculation methods resemble the methods used by the Board for the authorisation of plant protection products and biocides (Ctgb) to a great extent, it is not a tool to be used in the registration procedures. As local input with respect to climate, land use and timing of the application may highly influence the potential effects of the PPP, especially geographical information has been added to enlarge the evaluation capacity of the NMI.

### 2.1 Geographical information

The exposure concentrations as calculated by the NMI vary with both the time of application of the plant protection product (month of the application) and the location at which they are applied. Time influences the exposure concentrations because of temperature differences and differences in growth stage of the plants over the year. Because the parameters have spatial variability, the resulting exposure concentrations vary with space too. Characteristics of locations (x,y-coordinates) are stored into geographical databases, from which they are retrieved during the calculations.

In the STONE-instrument, a plot is defined by a unique combination of meteorology, physical and chemical soil conditions, boundary conditions for drainage flow, and boundary conditions for regional groundwater flow. The STONE-schematisation of the Netherlands has a resolution of 6.25 ha (250 x 250 m grid cells) and contains 6405 different plots (Kroon et al., 2001). An overlay was made of this national schematisation with the crop distribution maps (100 ha cell size (1 \* 1 km<sup>2</sup>), see section 2.5). So a NMI grid cell contains at maximum 16 STONE cells. Although in principle calculations are on a hectare basis and the NMI computes indicator units for each application of a plant protection product on an agricultural field, output is generated per grid cell.

## 2.2 Soil data

Soil characteristics (organic matter content, dry bulk density and pH) for each of the cells of  $1 * 1 \text{ km}^2$  were taken from the STONE instrument (Kroon et al., 2001). The original data, available at the  $250 * 250 \text{ m}^2$  scale were aggregated to the desired cell size. For the aggregation area weighted means over the 100 ha-cells were calculated.

## 2.3 Hydrological data

The NMI uses a metamodel of GeoPEARL for dividing the amount of PPP leaching downwards from the root zone (section 3.2.1) in two components; i) drainage flow of PPP towards the surface water, and ii) flow of PPP towards the groundwater. A prototype of GeoPEARL was used to calculate these two components for each STONE plot and for 20 combinations of PPP and application time (May, 15<sup>th</sup> or November, 1<sup>st</sup>). The median fraction of drainage flow is used for calculating the local emission by drainage flow towards surface water.

Aggregation of the median fraction of drainage flow depends on the seepage conditions:

1. if there is no upward seepage within the 100 ha-cell, the mean of the STONE grid cells (see section 2.1) is used to calculate lateral drainage flow;
2. if there is upward seepage in one or more STONE grid cells (see section 2.1) within the NMI grid cell, the area weighted national average lateral drainage flow is used to calculate the lateral drainage flow for the grid cell.

The density of surface watercourses within the NMI grid cells is based on the topographical map (TOP10-vector; scale 1 : 10000) and stored as the surface area ratio water : land per 100 ha-cell (assuming a constant water width of 1 m at all locations).

## 2.4 Climate data

For 15 meteorological regions daily average temperatures over a 20-year period (1981 – 2000) were provided by the Dutch Royal Meteorological Institute. Each grid cell in the STONE schematisation (see section 2.1) is assigned to one of the 15 meteorological stations. Monthly and yearly averages for NMI grid cells are calculated as the area weighted mean over the STONE cells within the NMI grid cell.

## 2.5 Crops

The crop definitions and crop areas in the NMI follow the classification system of Statistics Netherlands (CBS and LEI; 1998, 2004). In these statistics only the net arable land use surfaces are used, i.e. the agricultural land use without roads, edges and green borders (non-target crops). Depending on the application data available, these crops in the CBS-classification system can be included in the NMI. An NMI-crop is defined as a group of crops in the CBS-classification system. The resulting NMI-crop list contains 40 arable crops and 14 greenhouse crops including mushrooms (survey 1998). The total crop areas for both survey years are shown in Table 2.1.

The NMI-crop maps are calculated based on the crop statistics and on the land use map of the Netherlands (LGN4, LGN5; [www.lgn.nl](http://www.lgn.nl)). The land use map has a resolution of 25 \* 25 m<sup>2</sup>. The legend of the LGN contains nine agricultural land use classes; pasture, maize, potatoes, sugar beets, cereals, greenhouses, fruit orchards, flower bulbs and other crops besides several non-crop classes. The calculation procedure combines the detailed classification of municipality based crop statistics with the high resolution of the land use data:

1. aggregate each agricultural land use class from 25 m x 25 m pixels to a surface area per grid cell (in % per 100 ha);
2. relate each crop to an agricultural land use class;
3. distribute in each municipality the area of a crop among the grid cells containing the related land use class;
4. aggregate the area of CBS-crops to the area of NMI-crops per grid cell (in ha per 100 ha).

**Table 2.1 Data sources and summary data of the combination of crop statistics and land use for the two crop data sets in the NMI**

crop statistics (CBS)			land use data		NMI version 2		
survey (year)	number of municipalities	number of crops (CBS)	database version	satellite images (year)	number of crops (CBS) with application data available	number of NMI-crops	area covered with NMI-crops (%)
1998	540	123	LGN4	1999, 2000	69	54	95
2004	483	160	LGN5	2003, 2004	74	57	94

## 2.6 Plant protection product use data

Data on the use of plant protection products were obtained from databases of the Agricultural Economics Research Institute (LEI) and Statistics Netherlands (CBS), for the year 1998 and 2004. Both surveys were used to get the most reliable and national samples from a great range of pesticide uses in agriculture and horticulture. The survey of 2004 is almost entirely based on CBS data, because LEI data were not completely available. Pesticide use on grass was obtained from LEI because this was not covered by the CBS survey. Based on these surveys, the data are transformed from usage of plant protection products to active substances per crop per month. More details are given in Smidt et al. (2002).

The resulting data set provides information about:

- crop;
- active ingredient;
- (target) object;
- application method;
- month;
- dosage;
- number of applications per year;
- fraction treated area.

Table 2.2 gives some background information on the surveys of LEI and CBS.

**Table 2.2 Number of polls underlying the 1998 and 2004 use data sets**

sector	LEI 1998	CBS 1998	totals 1998	CBS 2004
arable farming	1344	165	1509	1112
bulbs	149	109	258	235
floriculture glasshouse	157	90	247	420
tree nursery	96	86	182	491
mushrooms	21	67	88	33
fruits	110	191	301	188
vegetables glasshouse	57	110	167	155
vegetables open air	199	61	260	569
cattle <sup>1</sup>	517	163	680	488
total	2650	1042	3692	3691

<sup>1)</sup> CBS 1998 only fodder maize

<sup>1)</sup> LEI 2004 grass survey

The NMI-database contains the average, annual dosage. The NMI is not prepared for handling regional based application data. For this reason, the usage of wet soil fumigants could not be included in the NMI-database.

Yearly sales data (the so-called RAG data), as gathered by the Dutch bureau 'Dienst BasisRegistratie', are used to adjust the above-mentioned LEI and CBS data so as to bring them in line with yearly total sales of each individual active substances. After editing (e.g. converting to active ingredient) the information on yearly sales of pesticides in the Netherlands is provided for use in the NMI by the Dutch Plant Protection Service.

Sales data include amounts of pesticides used by professionals on non-agricultural crops and other objects (for example sports grounds and pavements). As the NMI is intended to calculate emissions and effects from agricultural uses of plant protection products and calculation methods not necessarily are valid for non-agricultural uses of plant protection products, the sales data are corrected for the amounts used outside agriculture. Corrections were based on surveys as described by Syncera (2005).

The crop definitions (Appendix 3) and application data from the survey year 1998 are used for the calculations for the years 1998 - 2001, whereas the survey year 2004 is used for calculation years 2002 – 2005. This breakpoint between 2001 and 2002 more or less coincides with the implementation of the drift emission reduction measures according to the regulation ‘Lozingenbesluit Open Teelt en Veehouderij (LOTV)’.

## 2.7 Application techniques

Data on application techniques were also obtained from LEI and CBS. The data are gathered along with the use data in the previous paragraph. The data were grouped to enable the correct choice of the calculation method for the amount of pesticide emitted from the target area (Table 2.3). The way plant protection products are applied may affect the emission to environmental compartments and therewith the potential impact of the plant protection product.

**Table 2.3 Application techniques, emission routes and receiving environmental compartments**

object	application technique	environmental compartment and emission route				
		spray drift loss while application	volatilisation from crop, soil or hard surface	spray drift *	lateral drainage	runoff (point sources), leaching from casks, etc.
<i>field applications (whole field treatments):</i>						
crop	field spraying *	x	x	x	x	x
soil (surface)	field spraying *	x	x	x	x	x
	non-spraying		x		x	x
soil (mixing)	field spraying *	x		x		x
	non-spraying (granules)			x		x
<i>field applications (partial treatments):</i>						
crop	local spraying					x
stem	lubricating, aerosol			x		x
<i>in/near buildings:</i>						
bulb	dipping / disinfection				x	
crop root					x	x
stable	spraying				x	x
<i>greenhouses:</i>						
crop	spraying, fogging, LVM <sup>§</sup>		x	x <sup>^</sup>	x	x <sup>#</sup>
soil (surface)	spraying, fogging, LVM		x	x <sup>^</sup>	x	x <sup>#</sup>
soil (mixing)	spraying, granules, etc.			x <sup>^</sup>	x	x <sup>#</sup>

\* field spraying by a field sprayer in combination with drift reducing methods (see section 2.8)

<sup>^</sup> only for crops not cultivated on substrate

<sup>#</sup> only for crops not cultivated on substrate, in greenhouses without a pipe drainage system

<sup>§</sup> low volume mist application

Leaching to groundwater is calculated for all soil bound crops, both open air crops and greenhouse crops. Leaching is not calculated for crops grown on artificial substrates. For crops grown on both soil and artificial substrates, the fraction soil bound crop is used to calculate the leaching. Table 2.4 gives the soil bound fraction for these crops. Information is taken from the Geographical Information System for Agricultural Farms (GIAB) for the years 1998 and 2004.

If a plant protection product is sprayed over the crop, part of the dose may be intercepted by the crop. The percentage intercepted is dependent on the growth stage of the crop and the application technique. Appendix 4 gives the interception fractions, whereas Table 2.5 gives the extrapolation to crops not covered by the original data.

**Table 2.4 Greenhouse crops rooting in soil (fraction of the total crop area), the remaining part of the crop area is substrate**

crop	sector	survey year	
		1998	2004
freesias	floriculture (greenhouse)	0.96	1.00
lilies (glasshouse culture)		0.96	0.97
chrysanthemum		0.94	1.00
pot plants (green)		0.90	0.90
pot plants (flowers)		0.90	0.90
carnation		0.62	-
orchids		0.58	0.70
roses (glasshouse)		0.29	0.26
gerberas		0.25	0.23
alstroemeria		-	0.87
sweet pepper	glass vegetables (greenhouse)	0.08	0.17
cucumbers		0.07	0.15
tomatoes		0.06	0.15
radish		-	1.00

**Table 2.5 Extrapolation of interception fractions in the NMI**

reference crop	extrapolated to crop:
potatoes <sup>1</sup>	starch, ware and seed potatoes, tree nurseries, rose-bushes
apples <sup>1</sup>	apple trees, pear trees, fruit trees
beet <sup>1,5</sup>	sugar beet
chrysanthemum <sup>2</sup>	chrysanthemum, carnation, roses and other greenhouse flowers
trees <sup>1</sup>	trees, conifers
cereals <sup>1</sup>	bread wheat, spring barley, grass seed
lilies <sup>1</sup>	lilies, gladiola
fodder maize <sup>6</sup>	maize
spireas <sup>3</sup>	permanent plants
sprouts <sup>1,5</sup>	Brussels sprouts
tomatoes <sup>4</sup>	tomatoes, sweet pepper, cucumbers
tulips <sup>1</sup>	tulips, hyacinths, iris, daffodils
onions <sup>1</sup>	onions (bulbs), salsify, (seed) onions
vegetables <sup>5</sup>	asparagus, beans, cabbages, carrots and chicory
other <sup>5,7</sup>	strawberries, meadow, lettuce, spinach

<sup>1</sup> Van de Zande et al. (2000); <sup>2</sup> Tak (1995); <sup>3</sup> Van Kammen et al. (1998); <sup>4</sup> Bor et al. (1994);  
<sup>5</sup> MJP-G (1996); <sup>6</sup> Deneer et al. (1999), <sup>7</sup> expert judgment.

## 2.8 Drift

Spray drift data are stored in the NMI database, with different values for the two survey years. Drift data were constituted using four data sources:

- data on spraying equipment and spraying techniques, resulting from the surveys by Statistics Netherlands (see also section 2.6);
- spray drift data for standard spraying techniques under standard conditions, derived from research by Van de Zande et al. (1997) and Porskamp et al. (2001);
- spray drift reduction data resulting from measures to reduce spray drift to surface water;
- data on the degree of implementation of such measures in Dutch agriculture in 1998 (Wingelaar et al., 2001) and in 2004 (Vijftigschild, 2006)).

This information was used to construct drift tables. For the year 1998, standard spraying techniques were assumed (including standard no-spray zones) and standard spray drift factors were assigned to each combination of crop and application technique. For the year 2004, by regulation (LOTV; Kalf and Roex, 2003), Dutch farmers should apply drift reduction techniques when spraying plant protection

products in the open field. Minimum drift reductions percentages, resulting from these techniques, are given in the regulation. These reduction percentages were included in the drift tables for 2004. Often more than one application technique will be used to spray a specific plant protection product on a crop. Weighted average values are then used for the combination crop and PPP.

## **2.9 Substance fate and ecotox data**

For calculating environmental exposure a number of physico-chemical and fate data of plant protection products are necessary. The physico-chemical data include: molar mass, saturated vapour pressure and solubility in water. For acidic substances in addition the acid dissociation constant ( $pK_a$ ) is necessary. The fate data include: the constant for sorption on soil organic matter ( $K_{OM}$ ) (for acidic substances for both the molecular and the ionic species) and the transformation constant ( $DegT_{50}$ ) in soil under reference conditions. For metabolites essentially the same information is necessary and, in addition, the formation fraction, i.e. the molar fraction of the parent that is transformed into the metabolite. The ecotox data include  $LC_{50}$ ,  $EC_{50}$ ,  $LD_{50}$  and NOEC values for algae, birds, daphnia, earthworms and fish.

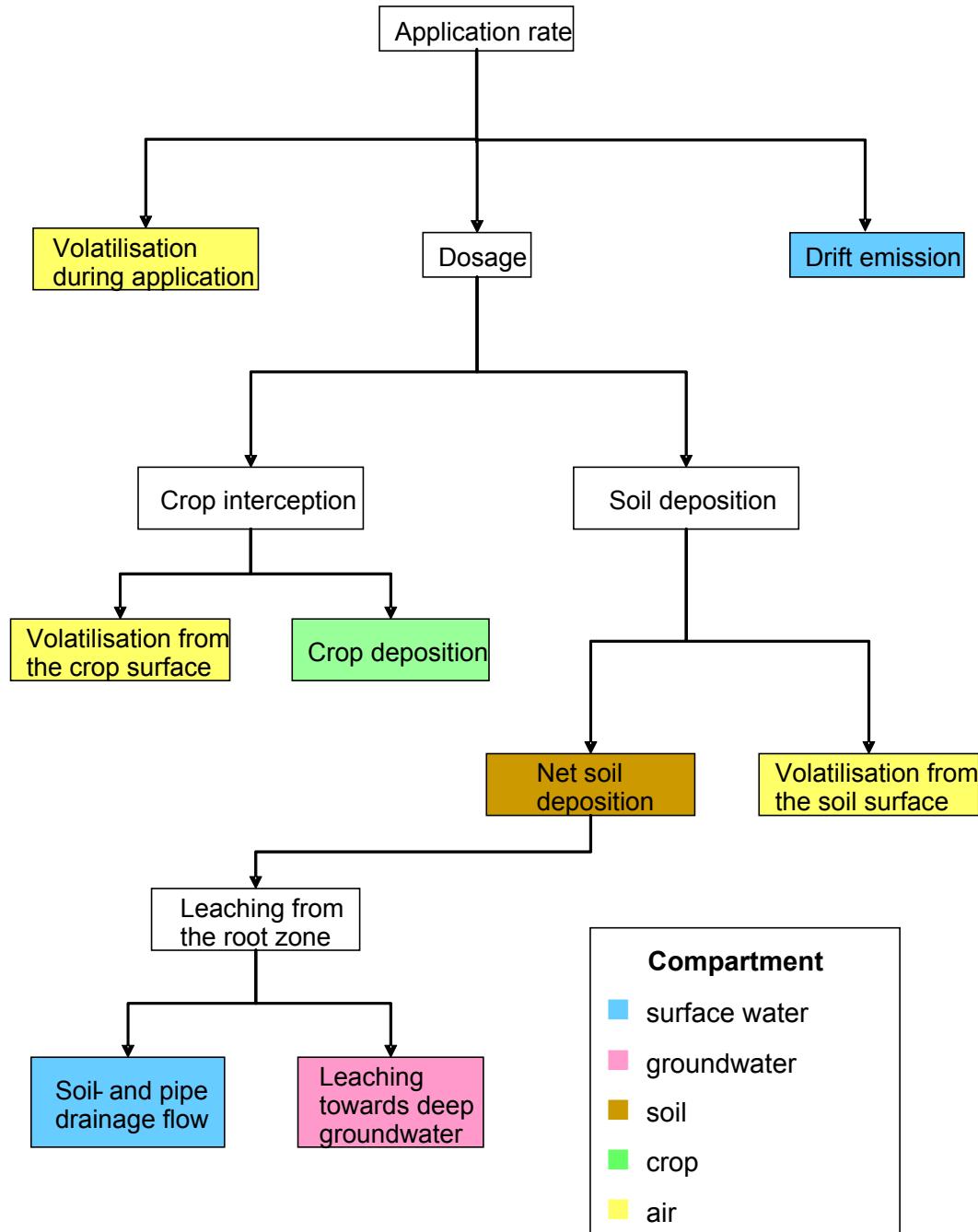
Appendix 5 gives a listing of all necessary substance fate and ecotox data as well as some miscellaneous data. Substance data need to be provided by the user of the instrument. The user should take care of providing data which are consistent with the requirements of the NMI. For easy reference units have been added to the table.

### 3 Emission indicators

One of the features of the NMI is that it can calculate emissions of plant protection products to non-target areas and compartments. The following non-target areas and compartments are distinguished:

- air
- groundwater;
- surface water;
- neighbouring nature areas.

This chapter describes the methods for calculating the emissions. Figure 3.1 gives an overview of included processes for open air applications. In general it is not possible to keep balance of all flows. The reason for this is that parameters for the individual processes are not always derived from experiments keeping balance of all processes. In contrary, often a single process is considered and parameters are related to the (nominal) dose applied in the experiment. For example, drift deposition onto surface water is expressed as the fraction (or %) of the nominal deposition on the target field per unit surface area (usually expressed in  $\text{mg m}^{-2}$ ), not as fraction of the total amount applied. As field dimensions are unknown, it is impossible to convert drift deposition fraction into absolute amounts.



Roel Kruijne, 15 november 2007

Figure 3.1 Overview of included processes for open air applications

### 3.1 Air

Volatilisation to air is calculated for three routes:

- volatilisation during application;
- volatilisation from plant leaves;
- volatilisation from the soil surface.

Volatilisation during application was studied by Holterman (2000); his results are included in the NMI:

$$E_{app,air} = f_{al} A \quad \text{Eq.3-1}$$

with:

$E_{app,air}$  emission to air during application, ( $\text{kg ha}^{-1}$ )  
 $f_{al}$  fraction of the dose lost during application, (-), default 0.03  
 $A$  the nominal rate for a single application, ( $\text{kg ha}^{-1}$ )

For a typical spray application on arable fields 3% of the applied amount stays in the air for a longer period and can be transported to outside the treated area. A part of the spray-droplets is or becomes so small that they stay air-born and their residence in the air is prolonged. The fraction volatilised during spraying when using an axial sprayer, as for instance in fruit cultivation and tree nurseries, might be higher. Data to support this assumption are lacking.

The volatilisation from plant leaves is calculated using the regression equation (Smit et al., 1998; Smidt et al., 2000):

$$\log(CV_{crop}) = 1.661 + 0.316 \log(P_{sat}) \quad \text{Eq.3-2}$$

with:

$CV_{crop}$  the cumulative volatilisation (% of amount reaching the crop)  
 $P_{sat}$  the saturated vapour pressure of the substance (mPa),  $P_{sat} \leq 11.8 \text{ mPa}$ .

The regression equation is based on a relatively small number of experiments.  $P_{sat}$  is dependent on the temperature (see Eq.3-3) and therefore the amount volatilised is dependent on the time and the place of application, which determine the temperature. If  $P_{sat} \geq 11.8 \text{ mPa}$  the cumulative volatilisation is taken to be 100%; substances having such a high  $P_{sat}$  are not likely to be sprayed on crops.

$$P_{sat} = P_{sat,r} \exp\left(\frac{-\Delta H_{vap}}{R} \left(\frac{1}{T} - \frac{1}{T_r}\right)\right) \quad \text{Eq.3-3}$$

with:

$P_{sat,r}$  the saturated vapour pressure at reference conditions, (mPa)  
 $\Delta H_{vap}$  molar enthalpy of vaporisation,  $\text{J mol}^{-1}$ , (value  $95000 \text{ J mol}^{-1}$ )  
 $R$  molar gas constant,  $(\text{J mol}^{-1} \text{ K}^{-1})$ , (value  $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ )  
 $T$  local temperature, (K)  
 $T_r$  reference temperature, (K), (value  $293.15 \text{ K}$ )

Eq.3-2 was derived for non-dissociating substances. Charged substances in general have a negligible tendency to volatilise. For weak acidic substances only the non-ionised form contributes to the volatilisation. For these substances, the volatilisation from the crop is corrected for the dissociation:

$$CV_{crop} = f_{ND,crop} CV_{crop} \quad \text{Eq.3-4}$$

with:

$$f_{ND,crop} = \frac{1}{1 + 10^{(pH_{app} - pK_a)}} \quad \text{Eq.3-5}$$

where:

$f_{ND,crop}$  the fraction not-dissociated substance on the leaf surface, (-)  
 $pH_{app}$  the pH of the application solution, (-), default  $pH_{app} = 7$   
 $pK_a$  the dissociation constant of the substance, (-)

For substances which become positively charged dependent on the pH (i.e. bases), in principle the volatilisation will become lower with declining pH. In databases, however, very few  $pK_a$  for such substances are recorded. Therefore the influence of pH on the volatilisation of these substances is neglected in the NMI. For inorganic substances almost never saturated vapour pressures are recorded in databases. For these substances, the saturated vapour pressure is set to zero and therefore the calculated volatilisation will be zero too.

The total amount of substance volatilised from the crop, assuming no wash-off from the plants, is calculated according to:

$$E_{crop,air} = \frac{CV_{crop} f_i (A - E_{app,air})}{100} \quad \text{Eq.3-6}$$

with:

$E_{crop,air}$  the total amount volatilised from the crop,  $(\text{kg ha}^{-1})$   
 $f_i$  fraction intercepted by the crop, (-), input from database  
 $100$  factor to convert from % to fraction

Volatilisation from the soil surface is also calculated using a regression equation (Smit et al., 1997; Smidt et al., 2000):

$$CV_{soil} = 71.9 + 11.6 \log(100 FP_{gas}) \quad \text{Eq.3-7}$$

in which  $CV_{soil}$  is the cumulative volatilisation from the soil surface (% of amount reaching the soil) and  $FP_{gas}$  is calculated from:

$$FP_{gas} = \frac{\varepsilon_{gas}}{\varepsilon_{gas} + \varepsilon_{liquid} K_{lg} + \rho_{soil} K_{lg} K_{sl}} \quad \text{Eq.3-8}$$

with:

- $FP_{gas}$  the fraction of substance in the gas phase, (-),  $0 \leq FP_{gas} \leq 1$
- $\varepsilon_{gas}$  the volumetric gas fraction, (volume gas per volume soil)
- $\varepsilon_{liquid}$  the volumetric liquid fraction, (volume soil solution per volume soil)
- $\rho_{soil}$  the soil dry bulk density, ( $\text{kg dm}^{-3}$ )
- $K_{lg}$  the liquid to gas partitioning coefficient, (-)
- $K_{sl}$  the soil to liquid partitioning coefficient, ( $\text{dm}^3 \text{kg}^{-1}$ ), (see Eq.3-16 and Eq.3-17)

The volumetric gas fraction is calculated according to:

$$\varepsilon_{gas} = I - \varepsilon_{liquid} - \varepsilon_{solid} \quad \text{Eq.3-9}$$

with:

$$\varepsilon_{solid} = \rho_{solid} / \rho_{solid} \quad \text{Eq.3-10}$$

and:

$$\rho_{solid} = I / (om_5 / \rho_{om} + (I - om_5) / \rho_{min}) \quad \text{Eq.3-11}$$

- $\varepsilon_{solid}$  the volumetric solid fraction, (volume solid parts per volume soil)
- $\rho_{solid}$  the density of the solid phase, ( $\text{g cm}^{-3}$  of soil)
- $om_5$  the organic matter fraction of the top 5 cm of the soil, (-)
- $\rho_{om}$  the density of organic matter, ( $= 1.47 \text{ g cm}^{-3}$  of soil)
- $\rho_{min}$  the density of mineral parts, ( $= 2.66 \text{ g cm}^{-3}$  of soil)

The liquid to gas partitioning coefficient,  $K_{lg}$ , is the inverse of the dimensionless Henry coefficient,  $K_H$  (-):

$$K_H = \frac{0.001 P_{sat} M}{R T_{gridcell} S} \quad \text{Eq.3-12}$$

with:

- M molar mass, (g mol<sup>-1</sup>)
- R molar gas constant, (8.314 J mol<sup>-1</sup> K<sup>-1</sup>)
- $T_{gridcell}$  temperature of the grid cell, (K)
- S solubility in water, (mg dm<sup>-3</sup>)
- 0.001 conversion factor from mPa to Pa

The Henry coefficient is dependent on the temperature as both the saturated vapour pressure (see Eq.3-3) and the water solubility are dependent on temperature:

$$S = S_r \exp\left(\frac{-\Delta H_{dis}}{R} \left(\frac{1}{T} - \frac{1}{T_r}\right)\right) \quad \text{Eq.3-13}$$

with:

- $S_r$  the solubility in water at reference temperature, (mg dm<sup>-3</sup>)
- $\Delta H_{dis}$  the molar enthalpy of dissolution, J mol<sup>-1</sup>, value 27000 J mol<sup>-1</sup>

Dissociation of substances also influences the partitioning of the substance over the three phases in the soil. For weak acidic plant protection products Eq.3-8 is modified to account for the dissociation of the substance:

$$FP_{gas} = \frac{\varepsilon_{gas}}{\left( \varepsilon_{gas} + \frac{\varepsilon_{liquid} K_{lg} + \rho_{soil} K_{lg} K_{sl}}{f_{ND,soil}} \right)} \quad \text{Eq.3-14}$$

with:

$$f_{ND,soil} = \frac{1}{1 + 10^{(pH_{gridcell} - pK_a)}} \quad \text{Eq.3-15}$$

where:

- $f_{ND,soil}$  the fraction not-dissociated substance in the soil surface layer, (-)
- $pH_{gridcell}$  the pH of the surface layer of the soil (upper 5 cm), (-), map information

The partitioning of the substance over the solid phase and the liquid phase is expressed by the partitioning coefficient  $K_{sl}$ , according to:

$$K_{sl} = om_5 K_{om} \quad \text{Eq.3-16}$$

and, for substances with pH-dependent sorption behaviour:

$$K_{sl} = om_5 K_{om,com} \quad \text{Eq.3-17}$$

with:

$K_{om}$  the organic matter sorption constant, ( $\text{dm}^3 \text{ kg}^{-1}$ )

$K_{om,com}$  the combined sorption constant, ( $\text{dm}^3 \text{ kg}^{-1}$ ), see Eq.3-27

The volatilisation from the soil surface is dependent on the time of application (as this influences temperature) and the location (as this determines temperature and soil type and, therefore,  $FP_{\text{gas}}$ ). The total amount volatilised from the soil surface, assuming no wash-off from the plants, is:

$$E_{soil,air} = \frac{CV_{soil} (1 - f_i) (A - E_{app,air})}{100} \quad \text{Eq.3-18}$$

with:

$E_{soil,air}$  the total amount volatilised from soil, ( $\text{kg ha}^{-1}$ )

100 factor to convert % to fraction

The total volatilisation (emission to air) for each substance is the sum of the individual volatilisation routes.

Except for soil fumigants, the amount of substance volatilised from the bulk soil usually is negligible and therefore not considered in NMI version 2. As stated earlier, soil fumigants are not included in the database of version 2 of the NMI.

Emissions from greenhouses by volatilisation to air is calculated based on the saturated vapour pressure of the substance and the application technique. Table 3.1 shows the volatilisation fraction for applications with high volume techniques, fogging and low volume techniques.

**Table 3.1 Volatilisation for combinations of vapour pressure class and application technique (fraction of the application rate)**

vapour pressure (mPa)	high volume	fogger	low volume
< 0.01	0.01	0.01	0.05
≥ 0.01 - < 0.1	0.05	0.05	0.15
≥ 0.1 - < 1	0.1	0.25	0.25
≥ 1 - < 10	0.3	0.35	0.35
≥ 10	0.4	0.4	0.4

## 3.2 Groundwater

The NMI calculates leaching to groundwater starting from the net soil deposition:

$$S_N = A - E_{app,air} - E_{crop,air} - E_{soil,air} - E_{sw,d} \quad \text{Eq.3-19}$$

with:

$S_N$  the net soil deposition, ( $\text{kg ha}^{-1}$ )  
 $E_{sw,d}$  emission to surface water as a result from drift, ( $\text{kg ha}^{-1}$ )

The nominal rate for a single application is obtained from the pesticide use table, which is based on pesticide use inventories by Statistics Netherlands (CBS) and the Agricultural Economics Research Institute (LEI) (see chapter 2.4). For a detailed description: see Smidt et al. (2002). The fraction washed off from the canopy is unknown; information is lacking and the (default) value is taken to be zero.

The leaching process is relatively slow compared to other emission processes and, therefore, transformation processes have to be taken into account when calculating emissions due to leaching. Transformation results in dissipation of a plant protection product and only a fraction of the net soil deposition will leach to groundwater. Transformation however also results in metabolites or other degradation products. (In the remainder of the text the term metabolites includes also other degradation products.) In principle, the NMI is capable of calculating the leaching of all metabolites, provided that the fate parameters of the metabolite and the relationship of the metabolite with a parent substance are included in the substances database. The relationship of parent and metabolite is indicated by a formation fraction, i.e. the amount of metabolite formed in mole equivalents of the parent. Also indirectly formed metabolites are related in this way to the parent. By including information on metabolites, the user of the NMI decides which metabolites are taken into account in the calculations.

The leaching of a substance is highly dependent on environmental conditions and chemical properties of the substance. The use of a generic leaching fraction is therefore not possible. Instead, a leaching fraction is calculated for each substance separately (see section 3.2.1) and this leaching fraction is used to calculate the leaching amount. The leaching to the depth of one metre below soil surface is calculated from:

$$E_{gw,p} = f_{fle} F_{PEARL} S_N \quad \text{Eq.3-20}$$

$$E_{gw,m} = f_{fle} \frac{M_m}{M_p} f_{p,m} F_{PEARL} S_N \quad \text{Eq.3-21}$$

with:

$E_{gw}$  predicted amount leaching to groundwater (depth one metre), ( $\text{kg ha}^{-1}$ )  
 $F_{PEARL}$  the leaching fraction obtained from the PEARL metamodel (see section 3.2.1), (-)  
 $M$  molar mass, ( $\text{g mol}^{-1}$ )  
 $f_{fle}$  factor to account for the fraction leaching error (see section 3.2.1), (-)  
 $f_{p,m}$  the molar fraction of the parent molecule converted to the metabolite, (-)  
 $p, m$  parent, respectively metabolite

The total amount leaching to groundwater at a depth of one metre is the sum of the amounts calculated for the parent and all relevant metabolites. For multiple applications the total amount reaching the soil is used to calculate the leaching. There is no correction for transformation of substances in between the applications. This is because transformation is already accounted for in the PEARL model; correction would lead to an overestimation of the transformation.

The net amount of pesticide arriving at the bottom of the unsaturated zone of the soil may be subject to further leaching to the deeper groundwater, but also subject to lateral drainage. The fractions lateral drainage to surface water ( $f_{dr}$ ) and leaching to groundwater ( $1-f_{dr}$ ) were calculated by running GeoPEARL for a number of representative substances and calculating the average of the fractions for each grid cell (see also section 2.3). The results were then stored as an attribute of the soil map and used in the calculations as appropriate. The amounts leaching to deeper groundwater are calculated as:

$$E_{dgw,p} = f_{fle} F_{PEARL} S_N (1 - f_{dr}) \quad \text{Eq.3-22}$$

and for metabolites as:

$$E_{dgw,m} = f_{fle} \frac{M_m}{M_p} f_{p,m} F_{PEARL} S_N (1 - f_{dr}) \quad \text{Eq.3-23}$$

with:

$E_{dgw}$  emission to deeper groundwater as a result of leaching, ( $\text{kg ha}^{-1}$ )  
 $f_{dr}$  fraction lateral drainage, (-), see section 2.3

The amounts going to surface water via lateral drainage,  $E_{sw,ld,p}$  and  $E_{sw,ld,m}$  are calculated analogously with  $(1-f_{dr})$  replaced by  $f_{dr}$ .

Leaching from greenhouses is calculated for soil bound crops (crops rooting in soil). Emissions to the groundwater is calculated when no drainage system is underlying the greenhouse. As it has been demonstrated that the leaching is underestimated by PEARL (Lieffijn et al., 2000) an additional leaching, proportional to the application rate is assumed. Emission by leaching from greenhouses therefore consists of i) a part depending on the physico-chemical properties of the substance (section 3.2.1), and ii) a fixed part of the application rate (0.1%).

### 3.2.1

#### Metamodel of PEARL

The NMI uses a metamodel of the PEARL model (Tiktak et al., 2000; Leistra et al., 2001) to calculate leaching to groundwater. The metamodel interpolates (logarithmically) between results obtained for standard runs with the PEARL model, using the half-life and the sorption constant of the plant protection product. The standard runs consisted of runs with the (former) standard Dutch scenario for variable half-life (range: 1 to 200 days), variable sorption constant (range: 0 to 200  $\text{dm}^3 \text{kg}^{-1}$ ) and variable application time (one for each month). A standard spray application of  $1 \text{ kg ha}^{-1}$  to the soil surface was assumed and volatilisation was switched off. The results, the maximum average concentration in the upper metre of the groundwater,  $C_{PEARL}$  ( $\text{mg m}^{-3}$  or  $\mu\text{g dm}^{-3}$ ), and the fraction leached to groundwater,  $F_{PEARL}$  (-), were transferred and stored into an NMI database. The metamodel is comparable with the method formerly used in pesticide registration (Linders and Jager, 1998).

Spatial variation in leaching is approximated by accounting for differences in temperature and differences in soil organic matter content in the grid cells. Differences in temperature are accounted for by calculating the local half-life for the plant protection product and using this local half-life in the interpolation procedure. The local half-life is calculated according to:

$$DegT_{50,l} = \frac{DegT_{50}}{f_T} \quad \text{Eq.3-24}$$

with:

$$f_T = \exp\left(\frac{-\Delta H_T}{R}\left(\frac{1}{T_{gridcell,lt}} - \frac{1}{T_{SS}}\right)\right) \quad \text{Eq.3-25}$$

with:

- $DegT_{50,l}$  the local half-life in the grid cell, (d)
- $DegT_{50}$  the nominal half-life of the substance as listed in the substance table, (d)
- $f_T$  factor denoting the influence of temperature, (-)
- $\Delta H_T$  molar enthalpy of transformation, ( $J \text{ mol}^{-1}$ ), (default value  $54000 \text{ J mol}^{-1}$ )
- $R$  molar gas constant, ( $J \text{ mol}^{-1} \text{ K}^{-1}$ ), (value  $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ )
- $T_{gridcell,lt}$  long term average temperature of the grid cell, (K)
- $T_{SS}$  long term average temperature of reference scenario, (K), (value  $282.36 \text{ K} \equiv 9.21 \text{ }^{\circ}\text{C}$ )
- The factor  $f_T$  is based on the long term average temperature because it accounts for the (relatively) small differences in temperature between the meteo districts in the Netherlands, while the day to day variations are already accounted for in the original calculations with PEARL.

The  $DegT_{50}$  is read from the NMI substance database. The  $DegT_{50}$  can be based on results from standard laboratory tests, but also on results from so-called higher tier experiments. The selection of the appropriate  $DegT_{50}$  is done outside the NMI; the NMI uses the value provided via the NMI substance database.

Differences in soil organic matter are accounted for by calculating local sorption constants. The local sorption constant of a substance in this approach is calculated from the sorption constant in the substance table and the organic matter content in the top 35 cm layer of the soil, which is dependent on the location:

$$K_{om,l} = \frac{om_{grid}}{om_{ref}} K_{om} \quad \text{Eq.3-26}$$

with:

- $K_{om,l}$  the local sorption constant, ( $\text{dm}^3 \text{ kg}^{-1}$ )
- $K_{om}$  the sorption constant from the substance table, ( $\text{dm}^3 \text{ kg}^{-1}$ )
- $om_{grid}$  the organic matter content in the top 35 cm layer of the grid cell, (%)
- $om_{ref}$  the organic matter content in the top layer of the reference, (4.7%)

The thickness of this layer originates from the STONE soil schematisation (see section 2.2). The organic matter content of the top 35 cm layer is chosen, because the majority of the transformation in

general takes place in the plough layer of the soil; transformation in deeper layer is usually less. The value of the reference organic matter content is according to the former Dutch Standard Scenario. The local sorption constant is used in the interpolation process.

In case of slightly acidic substances, there is a further correction for the pH of the grid cell. Firstly, a combined sorption constant for the acidic molecule and its conjugated base is calculated:

$$K_{om,com} = \frac{K_{om,acid} + \frac{(M-1)}{M} 10^{pH_{gridcell} - pK_a} K_{om,base}}{1 + \frac{(M-1)}{M} 10^{pH_{gridcell} - pK_a}} \quad \text{Eq.3-27}$$

with:

$K_{om,acid}$	the sorption constant of the acidic molecule, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$K_{om,base}$	the sorption constant of the conjugated base, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$M$	molar mass of the acidic molecule, ( $\text{g mol}^{-1}$ )
$pH_{gridcell}$	the pH of the top 35 cm of the grid cell soil, (-)
$pK_a$	the dissociation constant of the substance, (-)

Secondly, the local sorption of the substance is then calculated from:

$$K_{om,l} = \frac{om_{grid}}{om_{ref}} K_{om,com} \quad \text{Eq.3-28}$$

and this local sorption constant is used to interpolate in the metamodel. The procedure described above is identical for metabolites.

The  $K_{om}$ ,  $K_{om,acid}$  and  $K_{om,base}$  are read from the NMI substances database. The data may result from standard laboratory experiments as well as higher tier experiments. Again the user is responsible for providing the appropriate data to the NMI system.

For some substances, there might be evidence that PEARL – and consequently the metamodel – is not capable of predicting the correct leaching fraction. The pesticide registration procedure accounts for this incapability by using an error term ( $f_{le}$ ) in the calculation. The error term accounts for discrepancies in the leaching fraction, not for errors in the degradation and sorption constants. The fraction leaching error is to be provided via the NMI substances database; the default of this parameter is 1, indicating the absence of an error.

### 3.3 Surface water

The term surface water is used in two different senses in the Netherlands:

1. in pesticide registration, surface water is the water in watercourses that may be exposed to plant protection products;
2. in (overall) pesticide policy, surface water is defined as the body potentially holding water, i.e. the watercourse and its side-slopes.

When in pesticide policy reference is made to emissions to surface water, then the second definition is used; drift to watercourses contributes to these emissions. The two apprehensions have impact on the calculation routines in the NMI. To avoid confusion, in this report the term surface water will be used when referring to the first sense and the term watercourse for the second sense.

The total loss of pesticides by spray drift may partially be deposited on watercourses and surface water. Other areas on which spray drift may be deposited are: agricultural area outside the treated field, nature area and built-up area. In version 2 of the NMI the surface water is considered as the receiving area. The amounts entering the watercourse or the nature area can be calculated using appropriate values for the drift factors. The emission by drift to surface water is:

$$E_{sw,d} = \frac{A \%_{drift,sw} L_{sw} W_{sw}}{10^4 \cdot 100 \cdot 2} \quad \text{Eq.3-29}$$

with:

$E_{sw,d}$  the emission to surface water by the drift process, ( $\text{kg ha}^{-1}$ )

$\%_{drift,sw}$  the drift as influenced by application technique and drift reducing measures, (%), (see section 2.8)

$L_{sw}$  the length of the surface water (per ha field), (m)

$W_{sw}$  the width of the surface water, (m)

Note that the geometry of the treated field and the surface watercourses is not known.

The factors  $10^4$  and 100 in the denominator are to convert from  $\text{kg ha}^{-1}$  to  $\text{kg m}^{-2}$  and from % to fraction. The factor 2 in the denominator is to account for the wind direction: it is assumed that only surface water downwind from the treated area is exposed.

Another emission route of plant protection products to surface water is drainage. Water infiltrating in the soil may drain to surface water, sometimes via artificial drains. The emission of plant protection products to surface water via this route is calculated according to the method described in section 3.2.

The NMI also calculates various point source emissions from farm yards:

- emissions resulting from the treatment of plant materials (mainly flower bulb disinfection);
- emissions from mushroom cultivation (described in more detail in De Nie (2002));
- emissions to surface water resulting from cleaning glass of greenhouses;
- emissions from disposed artificial substrates;
- emissions due to disposal of surplus (drainage) water of greenhouses;
- emissions of condense water.

Except for the emission of condense water, the emissions mentioned above are assumed to be a fraction of the application rate:

$$E_{sw,tr} = f_{tr} \cdot A \quad \text{Eq.3-30}$$

with:

$f_{tr}$  fraction emitted to surface water, (-)

Eq.3.30 holds for all these individual emission routes (except emission of condense water).

The emission factors lump several factors influencing the overall emission from a specific source. For example, for the mushroom cultivation it takes into account the fraction of farms having a settling tank, the percentage of the dose reaching the settling tank and the dissipation from the settling tank by transformation and volatilisation. The emission factor for the emissions from flower bulb disinfection is 0.0014 (0.14%). Parameters determining the emissions from greenhouses are based on the GLAMI report (Lieffijn et al., 2000).

The fraction of the dose dissolved in the condense water depends on of the vapour pressure class of the substance and the crop height (Table 3.2). The height of the greenhouse crops is assumed constant in time (Table 3.3).

**Table 3.2 Fraction of dose solved in condense water**

saturated vapour pressure class (mPa)	crop height class (m)	fraction (-)
< 0.01	< 1	0.00005
< 0.01	> 1	0.00005
≥ 0.01 - < 0.25	< 1	0.0075
≥ 0.01 - < 0.25	> 1	0.0017
≥ 0.25 - < 10	< 1	0.036
≥ 0.25 - < 10	> 1	0.001
≥ 10	< 1	0.081
≥ 10	> 1	0.0046

**Table 3.3 Greenhouse crop height (m)**

<b>crop</b>	<b>sector</b>	<b>height (m)</b>
roses (glasshouse)	floriculture (greenhouse)	1.5
bed plants		1
pot plants (flowers)		0.5
chrysanthemum		0.5
freesias		0.5
gerberas		0.5
orchids		0.5
pot plants (green)		0.5
lilies (glasshouse culture)		0.5
carnation		0.5
alstroemeria		0.85
cucumbers	glass vegetables (greenhouse)	2
sweet pepper		2
tomatoes		2
radish		0.2
mushrooms	mushrooms	0.25

The total emission to surface water is the sum of the amounts from the drift process, the lateral drainage process and the emissions from point sources:

$$E_{sw} = E_{sw,d} + E_{sw,ld} + E_{sw,tr} + E_{sw,condens} \quad \text{Eq.3-31}$$

$E_{sw,tr}$  here is the sum of the emissions of all applicable point sources. Deposition of plant protection products from the air compartment is not considered in version 2 of the NMI.

## 4 Effect indicators

### 4.1 Soil

The general principle of comparing an exposure concentration with ecotoxicological data for organisms or the ecosystem is followed for the soil environment. Soil here is defined as the top layer of the treated field. For the thickness of this top layer the following default values apply:

- 0.05 m for spray applications when assessing acute and chronic risk;
- 0.05 m for injection applications, treated seeds, bulbs and tubers when assessing acute and chronic risk;
- 0.2 m for applications incorporated in soil when assessing acute and chronic risk.

The exposure concentration is calculated from the net soil deposition, soil characteristics obtained from the soil map of the Netherlands and, when relevant, the transformation rate of the substance.

#### 4.1.1 Soil exposure concentration, single application

Ecotoxicological data for soil organisms have the dimension  $[M\ M^{-1}]$  and therefore the exposure concentration also has the same dimension. Input to the calculation of the exposure concentration is the net soil deposition. The net soil deposition is calculated from the nominal application rate and several emission terms (see also Eq. 3.19):

$$S_N = A - E_{app,air} - E_{crop,air} - E_{soil,air} - E_{sw,d} \quad \text{Eq. 4-1}$$

All loss fractions play a role when a crop protection product is sprayed over the crop. When another application technique is used, for instance injection or incorporation, some of the loss fractions may be absent.

The nominal application rate and the loss fractions are derived from procedures as described in chapters 2 and 3. The fractions lost by volatilisation during application and drift depend on application technique and reduction measures as described elsewhere (Smidt et al., 2000; Smidt et al., 2002) and chapter 2). The fraction intercepted is dependent on the crop type and the growth stage of the crop, which in turn is dependent on the time (moment in the growth cycle). The fraction volatilised from the soil is dependent on physico-chemical properties of the crop protection product, soil characteristics, soil conditions and climate conditions (see section 3.1).

We may now convert the amount reaching the soil into a soil content to make an ecotoxicological assessment possible:

$$G = \frac{S_N}{10^4 d_{soil} \rho_{soil}} \quad \text{Eq.4-2}$$

with:

G the content of the substance in the soil resulting from one application, ( $\text{kg kg}^{-1}$ )  
 d<sub>soil</sub> the depth (thickness) of the soil layer, (m)

The dry bulk density is dependent on the soil type and therefore obtained from the soil map. The factor  $10^4$  is used to convert from  $\text{kg ha}^{-1}$  (the unit for application rates that is generally used) to  $\text{kg m}^{-2}$ .

Depending on the application type – spraying or incorporation - the depth over which the substance distributes is taken to be 5 or 20 cm. Usually, ecotoxicological data for soil organisms or soil functions are expressed as mg active ingredient per kg dry soil ( $\text{mg kg}^{-1}$ ). Conversion to these units invokes a factor of  $10^6$  in the numerator of the equation. The soil dry bulk density varies with soil type and ranges from approximately 1000 to 1500  $\text{kg m}^{-3}$  for mineral soils.

#### 4.1.2 Soil exposure concentration, multiple applications

If there is more than one application, the residues in soil may build up. A new application adds to the remains of the former application(s):

$$X_{TA} = X_R + G \quad \text{Eq.4-3}$$

with:

X<sub>TA</sub> the content in soil immediately after the last application, ( $\text{kg kg}^{-1}$ )  
 X<sub>R</sub> the content in soil immediately before the last application, ( $\text{kg kg}^{-1}$ ), the remains of former applications

The remains are calculated according to a (pseudo) first-order equation:

$$X_t = X_{TA} e^{-f_T k t} \quad \text{Eq.4-4}$$

with:

X<sub>t</sub> the content in soil at time t, ( $\text{kg kg}^{-1}$ )  
 k first order rate coefficient for transformation in soil, ( $\text{d}^{-1}$ )  
 t time (= time elapsed after last application), (d)  
 f<sub>T</sub> factor for the influence of temperature, the temperature is dependent on space and time, (-).

X can be expressed as a content, but also as an absolute amount. In a first-order rate equation, the transformation rate is independent of the concentration. As the soil bulk density is assumed constant for the top layer, the ratio between the amount in the soil and the soil content is constant. Usually the half-life (DegT<sub>50</sub>) of a substance is stored in databases. In the NMI half-lives for substances are stored in a substance table. The half-lives refer to standard conditions, i.e. 20 °C, top soil at pF2. The rate coefficient is calculated from the half-life according to:

$$k = \frac{\ln(2)}{\text{DegT}_{50,s}} \quad \text{Eq.4-5}$$

In most models, used for registration purposes, the transformation is dependent on soil temperature, soil moisture and depth in the soil profile. For the soil compartment in the NMI, depth is not relevant

because only the top layer of the soil is considered. In modern agriculture crops are irrigated when necessary; therefore the influence of soil moisture can be neglected as well. This leaves temperature as the only influencing factor. The influence of temperature is given by the Arrhenius equation:

$$f_T = \exp\left(\frac{-\Delta H_T}{R}\left(\frac{1}{T_{gridcell}} - \frac{1}{T_r}\right)\right) \quad \text{Eq.4-6}$$

with:

$T_{gridcell}$  the average monthly temperature of the grid cell, (K)

$T_r$  reference temperature, (K), (value 293.15 K  $\equiv$  20 °C, because of the requirements imposed on the substance database)

For acute assessments the peak content is used to compare with the ecotoxicological data for earthworms. Now the calculation of the peak content is not straightforward. The net deposition is not constant as one or several factors, for instance interception, may vary in time. Also temperature varies in time, causing the transformation to increase (raising temperature) or decrease (falling temperature). A numerical model has been built to calculate the peak content (amount). For all repeated applications, it is assumed that the interval period in between two applications is constant. The length of the interval period is obtained from the plant protection product use data (cf. section 2.6); the value is stored in a database. The result of the calculations, the soil content versus time, has the form of a saw-tooth line. The maximum content is taken for comparison with acute ecotoxicological data (see section 4.1.3) while the maximum time weighted average over a defined period is taken for comparison with chronic ecotoxicological data (section 4.1.4).

#### 4.1.3

#### Potential acute effects in soil

Toxicity data for soil organisms usually are expressed in  $\text{mg kg}^{-1}$ . The substance database contains  $\text{EC}_{50}$  or  $\text{LC}_{50}$  data for soil organisms or soil functions, expressed in  $\text{mg kg}^{-1}$ . These data are derived from standard experiments with soil organisms or soil samples. Before Environmental Indicator Units (EIU) can be calculated, the peak content has to be expressed in  $\text{mg substance per kg soil}$  (Eq.4-7). Next, if earthworm toxicity data are used for the calculation, the acute toxicity value has to be corrected for differences in the organic matter content of the soil in the grid cell and the organic matter content of the toxicity test soil (Eq.4-8).

$$\text{PIEC}_{soil} = 10^6 \cdot X_{TA} \quad \text{Eq.4-7}$$

with:

$\text{PIEC}_{soil}$  predicted initial environmental concentration in soil, ( $\text{mg kg}^{-1}$ )

$10^6$  conversion factor from  $\text{kg kg}^{-1}$  to  $\text{mg kg}^{-1}$ .

$$ECC_{soil,a} = EC_{50,s} \frac{OM\%_{gridcell}}{OM\%_{ref}} \quad \text{Eq.4-8}$$

with:

ECC <sub>soil,a</sub>	acute environmental concern concentration for the soil, (mg kg <sup>-1</sup> )
EC <sub>50,s</sub>	50% effect concentration for soil organism(s) under reference conditions (for brevity reasons only EC <sub>50</sub> is mentioned here, but other acute effect data might be used as well), (mg kg <sup>-1</sup> )
OM% <sub>gridcell</sub>	organic matter of the grid cell soil, (percentage)
OM% <sub>ref</sub>	organic matter of the (reference) test medium, (percentage) (default value 10 %)
	The adjustment based on the organic matter content of the grid cell acknowledges that the pore water concentration is more important for the ecotoxicity than the total content.

The number of Environmental Indicator Units is now calculated from:

$$EIU_{soil,a} = \frac{PIEC_{soil}}{ECC_{soil,a}} \quad \text{Eq.4-9}$$

with:

EIU<sub>soil,a</sub> environmental indicator units for soil for the acute situation, (-).

Sometimes assessment factors are used in the authorisation procedure of plant protection products. The NMI does not explicitly account for assessment factors. If for some reason an assessment factor has to be applied, an adjusted toxicity value (EC<sub>50</sub>) has to be provided in the database.

#### 4.1.4 Potential chronic effects in soil

The substance database contains NOEC data for soil organisms and / or soil processes in mg kg<sup>-1</sup>. These data are derived from standard experiments with soil organisms or soil samples. The calculation of potential chronic effects requires the calculation of a time weighted average of the soil content (Eq.4-10) and the conversion of the chronic toxicity data to reference condition cell and the organic matter content of the toxicity test soil (Eq.4-11). Eq.4-10 is for a single application; for multiple application the maximum of the TWA is required. In the NMI code this is calculated via a numerical procedure.

$$TWA_{soil} = \frac{1}{t_{exp}} \int_0^{t_{exp}} PIEC_{soil} e^{-f_{soil,T} k_{soil} t} dt = \frac{PIEC_{soil} (1 - e^{-f_{soil,T} k_{soil} t_{exp}})}{f_{soil,T} k_{soil} t_{exp}} \quad \text{Eq.4-10}$$

with:

TWA<sub>soil</sub> Time Weighted Average environmental concentration in soil, (mg kg<sup>-1</sup>)  
 t<sub>exp</sub> appropriate exposure time, depending on the soil organism under consideration, (d)

$$ECC_{soil,c} = NOEC_s \frac{OM\%_{gridcell}}{OM\%_{ref}} \quad \text{Eq.4-11}$$

with:

ECC<sub>soil,c</sub> chronic environmental concern concentration for the soil, (mg kg<sup>-1</sup>)  
 NOEC<sub>s</sub> no observed effect concentration for soil organism under reference conditions, (mg kg<sup>-1</sup>);  
 OM%<sub>gridcell</sub> organic matter of the grid cell soil, (percentage)

OM%<sub>ref</sub> organic matter of the (reference) test medium, (percentage) (default value 10 %)  
 The adjustment based on the organic matter content of the grid cell acknowledges that the pore water concentration is more important for the ecotoxicity than the total content.

The number of Environmental Indicator Units is now calculated from:

$$EIU_{soil,c} = \frac{TWA_{soil}}{ECC_{soil,c}} \quad \text{Eq.4-12}$$

with:

EIU<sub>soil,c</sub> environmental indicator units for soil for the chronic situation, (-).

As for the acute situation, the NMI does not explicitly provide for taking assessment factors into account. If necessary, an adjusted toxicity value (NOEC) has to be provided in the database.

## 4.2 Groundwater

The general principle of comparing an exposure concentration with ecotoxicological data for organisms or the ecosystem is not followed for the groundwater environment; instead the threshold value for pesticides in drinking water is used. Groundwater here is defined as the water present in the top meter of the saturated zone beneath the treated field. In general there is some time lapse in between the application of the pesticide and the occurrence of the substance in groundwater. Therefore, the groundwater indicator is regarded as a chronic indicator. As described in section 3.2, the NMI uses a metamodel of the PEARL model for these calculations. Instead of leached amounts the concentration of the plant protection product or its relevant metabolites in the uppermost groundwater is used.

### 4.2.1 Groundwater exposure concentration

The drinking water threshold level as well as an ecological effect concentration has the dimension of concentration [M L<sup>-3</sup>] and therefore the exposure concentration should also have the same dimension. Therefore, an analogous procedure to the calculation of leaching emission (see sections 3.2 and 3.2.1) is used. Instead of a fraction leached to groundwater, now the resulting concentration in the groundwater is used. In the procedure the fraction leached (F<sub>PEARL</sub>) is replaced by the concentration (C<sub>PEARL</sub>):

$$PEC_{gw,p} = f_{fle} C_{PEARL} S_{N,T} \quad \text{Eq. 4-13}$$

$$PEC_{gw,m} = \frac{M_m}{M_p} f_{fle} f_{p,m} C_{PEARL} S_{N,T} \quad \text{Eq. 4-14}$$

with:

PEC<sub>gw</sub> predicted environmental concentration in groundwater, (µg dm<sup>-3</sup>)

C<sub>PEARL</sub> the concentration obtained via interpolation in the PEARL metamodel, (µg dm<sup>-3</sup>)

S<sub>N,T</sub> the total net soil load, (kg ha<sup>-1</sup>)

If there is more than one metabolite, the calculation is repeated for each metabolite. The conversion fractions ( $f_{p,m}$ ) always relate the metabolite to the parent, also when the conversion is via other metabolites. Note that this procedure is different from the procedure in the PEARL model; there second generation metabolites are related to the first generation metabolites, and so on.

#### 4.2.2 Potential effects in groundwater

As it usually takes some time before substances reach groundwater and the residence time of substances in groundwater is rather long, effects in groundwater are considered chronic effects. Environmental Indicator Units are derived from the comparison of the groundwater exposure concentration,  $PEC_{gw}$ , with a groundwater environmental concern concentration. An example of a groundwater environmental concern concentration is the threshold level for substances in drinking water of  $0.1 \mu\text{g dm}^{-3}$ :

$$EIU_{gw} = \frac{PEC_{gw}}{ECC_{gw}} \quad \text{Eq. 4-15}$$

with:

$EIU_{gw}$  environmental indicator units for groundwater, (-)

$ECC_{gw}$  environmental concern concentration for a substance in groundwater, ( $\mu\text{g dm}^{-3}$ )

This calculation is repeated for each of the relevant metabolites and the  $EIU_{gw}$  are summed to give the final potential effect of the application.

### 4.3 Surface water

The general principle of comparing an exposure concentration with ecotoxicological data for organisms or the ecosystem is followed for the surface water environment. Surface water in the current version of the NMI is assumed to be a water body with a surface width of 1 m, a depth of 0.3 m and slopes of 45 degrees. So per  $\text{m}^2$  water surface the water content of the surface water body is  $0.21 \text{ m}^3$  ( $210 \text{ dm}^3$ ). The length of the water bodies varies from grid cell to grid cell; the length is taken into account in the calculation of EIUs's.

The exposure concentration is calculated from the drift deposition, which in turn is dependent on application technique, crops factors and emission reduction measures. EIUs can be calculated for algae, daphnids, fish or the aquatic system as a whole. For which species EIUs are calculated is dependent on the ecotoxicity data provided via the NMI database.

Because little is known about the pattern (spatial, temporal) of the emissions from greenhouses towards the surface water, the resulting environmental effects cannot be estimated. These emissions are not yet converted to exposure concentrations in surface water.

#### 4.3.1 Surface water acute exposure concentration, single application

Ecotoxicological data for surface water organisms have the dimension [ $\text{M L}^{-3}$ ] and therefore the exposure concentration should be expressed in the same dimension. Input to the calculation of the

exposure concentration is the net surface water deposition. This surface water deposition is calculated from the nominal application rate and a drift factor:

$$S_{sw} = f_{d,sw} A \quad \text{Eq.4-16}$$

with:

$S_{sw}$  the net surface water deposition, ( $\text{kg ha}^{-1}$  (surface water))  
 $f_{d,sw}$  fraction drift to surface water, (-)

The drift factor indicates the deposition of spray drift averaged over the width of the water body. Note that  $f_{d,sw}$  is different from  $f_d$  mentioned in Eq.4-1. The initial concentration in the surface water can now be calculated from the dimensions of the water body and the net surface water deposition:

$$PIEC_{sw} = \frac{S_{sw}}{10 \left( W_{sw} d_{sw} - \frac{d_{sw}^2}{\tan \alpha} \right)} \quad \text{Eq.4-17}$$

with:

$PIEC_{sw}$  the initial concentration in surface water immediately after application, ( $\text{mg dm}^{-3}$ )  
 10 conversion factor from  $\text{kg ha}^{-1}$  to  $\text{g m}^{-2}$   
 $W_{sw}$  width of the surface water (wet surface), m  
 $d_{sw}$  depth of the surface water, m  
 $\alpha$  acute angle of the slope of the ditch with the soil surface

#### 4.3.2 Surface water acute exposure concentration, multiple applications

If there is more than one application, the residues in surface water may build up. A new application adds to the remains of the former application(s):

$$S_{sw,ta} = S_{sw,r} + S_{sw} \quad \text{Eq. 4-18}$$

with:

$S_{sw,ta}$  the amount in surface water immediately after the last application, ( $\text{kg ha}^{-1}$ )  
 $S_{sw,r}$  the amount in surface water immediately before the last application, ( $\text{kg ha}^{-1}$ ), the remains of former applications

The remains are calculated according to a first-order equation:

$$S_{sw,t} = S_{sw,ta} e^{-f_{sw,T} k_{sw} t} \quad \text{Eq. 4-19}$$

with:

$S_{sw,t}$  the amount in surface water at time  $t$  (= time elapsed after last application), ( $\text{kg ha}^{-1}$ )  
 $k_{sw}$  first order rate coefficient for dissipation from surface water, ( $\text{d}^{-1}$ )  
 $t$  time, (d)  
 $f_{sw,T}$  factor for the influence of the temperature of the surface water body, (-).

Several processes may contribute to the dissipation from surface water. The NMI accounts for two processes: degradation in the water system and volatilisation from the water system. In the NMI half-lives for substances are stored in a substance table. The half-lives refer to standard conditions, i.e. 20 °C. The rate coefficient for degradation in the surface water is calculated using Eq.4-5, in which the DegT<sub>50</sub> for the soil compartment is replaced by the transformation half-life in surface water (DegT<sub>50,sw</sub>). Temperature effects are accounted for using Eq.4-6.

Volatilisation from surface water is calculated according to:

$$k_{vol} = \frac{W_{sw}}{V_{sw}} \left( \frac{1}{K_l} + \frac{1}{K_g K_H} \right)^{-1} \quad \text{Eq.4-20}$$

with:

$k_{vol}$	volatilisation rate coefficient, (d <sup>-1</sup> )
$W_{sw}$	width of the water surface in the standard ditch, (1 m)
$V_{sw}$	volume of water per m length of standard ditch, (0.21 m <sup>2</sup> )
$K_l$	transport coefficient in the water phase, (2 m d <sup>-1</sup> )
$K_g$	transport coefficient in the gas phase, (200 m d <sup>-1</sup> )
$K_H$	dimensionless Henry coefficient, (-), (Eq.3-12)

The saturated vapour pressure is adjusted for the temperature in the grid cell, using for all substances a molar enthalpy of vaporisation of 95000 J mol<sup>-1</sup>. The solubility in water is adjusted for the temperature in the grid cell, using for all substances a molar enthalpy of solution in water of 27000 J mol<sup>-1</sup>.

The first order rate coefficient for dissipation from surface water is calculated as the sum of the rate coefficient for transformation and the rate coefficient for volatilisation:

$$k_{sw} = k_{sw,deg} + k_{sw,vol} \quad \text{Eq.4-21}$$

For acute assessments a peak concentration is used to compare with the ecotoxicological data. Now the calculation of the peak concentration is not straightforward. The net deposition is not constant as one or several factors influencing drift may vary in time. Also temperature may change, causing the dissipation rate to increase (raising temperature) or decrease (falling temperature). A numerical model has been built to calculate the peak concentration. The time between two applications is assumed constant for a given substance / crop combination. The time interval is derived from plant protection use data (cf. section 2.6). The time interval is stored in a database and used in the calculations, as appropriate.

The initial concentration in the surface water can now be calculated from the dimensions of the water body and the net surface water deposition (see also Eq.4-17):

$$PIEC_{sw} = \frac{S_{sw,ta}}{10 \left( w_{sw} d_{sw} - \frac{d_{sw}^2}{\tan \alpha} \right)} \quad \text{Eq.4-23}$$

A time weighted average concentration for chronic evaluation can be calculated from:

$$TWA_{sw} = \frac{1}{t_{exp}} \int_0^{t_{exp}} PIEC_{sw} e^{-f_{sw,T} k_{sw} t} dt = \frac{PIEC_{sw} (1 - e^{-f_{sw,T} k_{sw} t_{exp}})}{f_{sw,T} k_{sw} t_{exp}} \quad \text{Eq. 4-24}$$

In the NMI code is solved numerically.

#### 4.3.3 Potential acute effects in surface water

The calculations in sections 4.3.1 and 4.3.2 give results for surface waters receiving a drift deposition, expressed as an amount per unit area surface water. In general only surface water leeward to the treated field will receive spray drift. The standard spray drift factors (as laid down in the drift table) are derived from field experiments on spray drift in which the wind direction was perpendicular to the surface water, with a tolerance of 30 degrees in either direction (Van de Zande et al., 2000) and the surface water leeward to the treated field. Surface water in the windward direction does not receive spray drift. When in practice the wind has a smaller angle with the surface water, the spray drift deposition may be overestimated.

A second factor, which is important in the calculation of the EIUs, is the length of the surface water body along the treated field. In pesticide registration in the Netherlands the length of the water body determines the number of applications that are considered in the calculation of the peak concentration. As the (fixed) length of the ditch is 320 m and the rate of the water flow is 10 m per day (in spring), a limited number of applications – depending on the application interval - is considered. The NMI disregards this limitation and considers all applications. Still, the length plays an important role as it is a measure of the total volume of water exposed to the substance. In the NMI calculations the length is incorporated relatively to the length of the surface water in a reference situation.

The EIUs for surface water are now calculated according to:

$$EIU_{sw,a} = \frac{f_w f_{DL} PIEC_{sw}}{ECC_{sw,a}} \quad \text{Eq.4-25}$$

with:

$EIU_{sw,a}$	Environmental Indicator Units for surface water, acute, (-)
$f_w$	factor accounting for wind direction, (-, default 0.5)
$f_{DL}$	factor accounting for ditch length, depending on map information, (-)
$ECC_{sw,a}$	environmental concern concentration for surface water, acute, ( $\text{mg dm}^{-3}$ )

The factor  $f_{DL}$  accounts for differences in the lengths of ditches in a cell as compared to the length of ditches in a reference cell.

Also the  $ECC_{sw,a}$  is provided to the calculations via a database. The user has to choose between surface water organisms or the aquatic ecosystem and provide the database with the appropriate data. For example, the user can choose to supply data for:

- 1 algae,  $ECC_{sw,a}$  is then equal to the  $EC_{50}$  for algae ( $EC_{50,algae}$ );

- 2 daphnids,  $ECC_{sw,a}$  is then equal to the  $LC_{50}$  for daphnids ( $LC_{50,daphnids}$ );
- 3 fish,  $ECC_{sw,a}$  is then equal to the  $LC_{50}$  for fish ( $LC_{50,fish}$ );
- 4 the aquatic ecosystem,  $ECC_{sw,a}$  is then equal to the lowest of the three  $EC_{50}$  or  $LC_{50}$  values mentioned above.

If assessments factors are necessary, the toxicity values have to be adjusted using appropriate assessment factors and the adjusted values have to be stored in the NMI database.

#### 4.3.4 Potential chronic effects in surface water

Chronic effects in surface water are calculated by comparing an appropriate TWA concentration with chronic toxicity data for surface water organisms:

$$EIU_{sw,c} = \frac{f_w f_{DL} TWA_{sw}}{ECC_{sw,c}} \quad \text{Eq.4-26}$$

with:

$EIU_{sw,c}$	Environmental Indicator Units for surface water, chronic, (-)
$ECC_{sw,c}$	environmental concern concentration for surface water, chronic, ( $\text{mg dm}^{-3}$ )

The  $f_{DL}$  accounts for differences in the lengths of ditches in a cell as compared to the length of ditches in a reference cell.  $AF_{sw,c}$  depends on the exact nature of the calculations and is provided to the calculations via a database. The values are calculated off-line.

Also the  $ECC_{sw,c}$  is provided to the calculations via a database. The user has to choose between surface water organisms or the aquatic ecosystem and provide the database with the appropriate data. For example, the user can choose to supply data for:

- 1 algae,  $ECC_{sw,c}$  is then equal to the NOEC for algae ( $NOEC_{algae}$ );
- 2 daphnids,  $ECC_{sw,c}$  is then equal to the NOEC for daphnids ( $NOEC_{daphnids}$ );
- 3 fish,  $ECC_{sw,c}$  is then equal to the NOEC for fish ( $NOEC_{fish}$ );
- 4 the aquatic ecosystem,  $ECC_{sw,c}$  is then equal to the lowest of the three NOEC values mentioned above.

If assessments factors are necessary, the toxicity values have to be adjusted using appropriate assessment factors and the adjusted values have to be stored in the NMI database.

### 4.4 Terrestrial organisms

For the environmental indicator the partridge (body weight 370 g) is chosen as standard species, because birds are generally more sensitive than mammals and partridges are known to forage in field margins. It is assumed that the diet consists of 22% short grass, 21% leaves, 38.5% small seeds, 6.5% cereals and 12% small insects. Furthermore calculations are with fresh weight data for food.

For the moment only potential impact of sprayed PPP are included in the NMI; potential impacts of seed dressings, injected or incorporated and granular applications will be added later.

#### 4.4.1 Dietary exposure of birds and mammals by sprayed pesticides

The exposure of birds and mammals feeding on treated fields is calculated on the basis of the food consumption of the animals and the applied amount of plant protection product. As most toxicological experiments are performed using the nominal dosage, this dosage is used in the calculation. The daily chemical intake (DCI) for birds and mammals can be calculated with:

$$DCI = \frac{DEE}{\left( FE \left( 1 - \frac{MC}{100} \right) \frac{AE}{100} \right)} \frac{RUD}{1000} A f_{AV} f_{TWA} \quad \text{Eq.4-27}$$

with:

- DCI daily chemical intake, ( $\text{mg d}^{-1}$ ), (per unit dose of 1 kg active substance per hectare)
- DEE daily energy expenditure, ( $\text{kJ d}^{-1}$ )
- FE food energy, ( $\text{kJ}$  per dry gram food)
- MC moisture content of the food, (%)
- AE assimilation efficiency, dependent on the species, (%)
- RUD Residue unit dose (mg per kg fresh weight food per unit dose of 1 kg active substance per hectare)
- A dosage ( $\text{kg ha}^{-1}$ )
- $f_{AV}$  avoidance factor (-, 1 = no avoidance, 0 = complete avoidance)
- $f_{TWA}$  Time Weighted Average fraction (-, default is no degradation for acute exposure and 0.53 for long term exposure ( $DT_{50}$  of 10 days))

The DEE is different for birds and mammals and for the latter a distinction is made between rodents (no desert species) and other mammals (not including sea and desert species) (see Table 4.1). It is not necessary to differentiate between passerines and non-passerines, because the difference between the two groups is negligible.

**Table 4.1 Daily energy expenditure (DEE) for different groups of birds and mammals (calculated with data provided by Nagy, 1987)**

group	DEE ( $\text{kJ d}^{-1}$ )
rodents (no desert species)	$10^{(0.8685+0.6935 \log(BW))}$
other mammals (eutherians; excluding sea and desert species and rodents)	$10^{(0.7789+0.7007 \log(BW))}$
birds (all)	$10^{(1.019+0.6809 \log(BW))}$

Note: BW (body weight) in grams

Table 4.2 presents average RUD values for several types of food (after Luttkik et al., 2001). The RUD for long-term exposure assessments are based on the 50<sup>th</sup> percentile of residue data and for short term exposure assessments on the 90<sup>th</sup> percentile of these data (realistic worst case assumption).

**Table 4.2 Residue unit dose (RUD) values (mg kg<sup>-1</sup> fresh weight food) for an application rate of 1 kg ha<sup>-1</sup> (after Luttk et al., 2001)**

food type	food code	RUD for medium and long term exposure (= 50 <sup>th</sup> percentile)	RUD for acute/short term exposure (= 90 <sup>th</sup> percentile)
short grass	F1	61.6	142
long grass	F2	21.3	69
leaves	F3	25	87
leafy crops	F4	25	87
forage crops	F5	25	87
small seeds	F6	25	87
fruit	F7	2.3	11
pods	F8	2.3	11
large seeds	F9	2.3	11
small insects (foliar application)	F10	25	87
large insects (foliar application)	F11	2.7	11
insects (soil application)	F12	0.1	1

Table 4.3 lists the moisture content, the energy content and the assimilation efficiency for birds as well as for mammals for the same types of food.

**Table 4.3 Moisture content, energy content, assimilation efficiency for different types of food for birds and mammals**

food type	food code	moisture content, %	energy content, kJ g <sup>-1</sup> (dw)	assimilation efficiency, % (mammals)	assimilation efficiency, % (birds)
short grass	F1	76.4	18	46	37.2
long grass	F2	76.4	18	46	37.2
leaves	F3	88.6	11.2	74	76
leafy crops	F4	88.6	11.2	74	76
forage crops	F5	82.1	18	74	76
small seeds	F6	11.9	21	83	78.7
fruit	F7	83.7	11.6	74	55.8
pods	F8	11.9	21	83	78.7
large seeds	F9	13.3	16.7	83	78.7
small insects (foliar application)	F10	70.5	21.9	88	72
large insects (foliar application)	F11	70.5	21.9	88	72
insects (soil application)	F12	70.5	21.9	88	72

The data and formula presented so far allows one to calculate the daily chemical intake for one single food item. The daily diet of most species consists of several kinds of food, so the calculation becomes more complicated. For instance the average dietary fractions of a partridge are 0.22 for short grass, 0.21 for leaves, 0.385 for small seeds, 0.065 for large seeds and 0.12 for small insects. These values can not be used directly in connection with the DEE. First the metabolisable energy in 1 kg food has to be calculated:

$$ME_{tot} = \sum_{i=1}^{12} 1000 F_i 0.01 AE_i (1 - 0.01 MC_i) FE_i \quad \text{Eq.4-28}$$

with:

$ME_{tot}$  the total metabolisable energy, (kJ)

$i$  food type

$F$  fraction of food type I in diet

1000 factor to convert kilogram to gram

0.01 factor to convert % to fraction

Equation 4-28 can be used for all animals, i.e. birds, rodents and other mammals (see Table 4.1), by choosing appropriate values for the assimilation energy. The total metabolisable energy of the food can be used to calculate the Daily Food Intake (DFI) for a certain species in g (ww) per day:

$$DFI = \frac{1000 DEE}{ME_{tot}} \quad \text{Eq.4-29}$$

The Daily Chemical Intake can be calculated according to:

$$DCI_{tot} = \sum_{i=1}^{12} \frac{A F_i ME_{tot} RUD_i f_{AV,i} f_{TWA,i}}{1000} \quad \text{Eq.4-30}$$

by choosing appropriate values for acute or chronic RUD values and avoidance factors. The  $f_{TWA}$  is only to be used when assessing potential chronic effects.

In Appendix 6 the default values for the dietary exposure model due to sprayed products are presented. With the general model one will be able to calculate exposure concentrations for most birds and mammals in the Netherlands or Europe.

#### 4.4.2

#### Potential effects for the terrestrial ecosystem

For the NMI the partridge has been chosen as standard species. A bird species is chosen because in general birds are more sensitive to pesticides than mammals and / or the exposure is higher for birds than for mammals (a bird of 100 gram needs 1.6 times more energy than a mammal having the same body weight). A partridge is used because this species is known to forage in the field margins. The text box below gives some characteristic results for the partridge.

**Characteristic data for the partridge**

The general data necessary for calculating the acute exposure and the long term exposure of a partridge to a pesticide are: it is a bird with a body weight of 370 grams, the diet consists of 22% short grass, 21% leaves, 38.5% small seeds, 6.5% cereals and 12% small insects (see also column 2 of Table A1), no avoidance is assumed and the default value for  $f_{TWA}$  is appropriate. For the calculations an application rate of 1 kg ha<sup>-1</sup> was assumed.

**Output**
**Acute exposure**

Daily energy expenditure	DEE	585.7 kJ
Assimilation efficiency corrected DFI	DFI (ww) +AE	78.6 g d <sup>-1</sup>
Daily chemical intake	DCI (ww)	7.4 mg d <sup>-1</sup>

**Long term exposure**

Daily energy expenditure	DEE	585.7 kJ
Assimilation efficiency corrected DFI	DFI (ww) +AE	78.6 g d <sup>-1</sup>
Daily chemical intake	DCI (ww)	1.3 mg d <sup>-1</sup>

The potential acute effect for the terrestrial ecosystem is now calculated according to:

$$EIU_{te,a} = \frac{1000 DCI_{tot,a} A}{LD_{50,te} BW} \quad \text{Eq.4-31}$$

with:

- $EIU_{te,a}$  Environmental Indicator Units for the terrestrial ecosystem, acute, (-)
- 1000 factor for the conversion kg to g
- A the nominal application rate, (kg ha<sup>-1</sup>)
- $DCI_{tot,a}$  the acute total chemical intake, (mg per unit dose of 1 kg active substance per hectare) )
- $LD_{50,te}$  the lethal dose 50% for the selected organism, (mg kg<sup>-1</sup>)
- BW the body weight of the animal, (g)

Like in the other compartments, an assessment factor might be necessary. In such a case, the user has to supply adjusted data for the toxicity.

Chronic effects for the terrestrial ecosystem are calculated from:

$$EIU_{te,c} = \frac{1000 DCI_{tot,c} A}{NOEC_{te} BW} \quad \text{Eq.4-32}$$

with:

- $EIU_{te,c}$  Environmental Indicator Units for the terrestrial ecosystem, chronic, (-)
- 1000 factor for the conversion kg to g

DCI<sub>tot,c</sub> the chronic total daily chemical intake, (mg d<sup>-1</sup>, per unit dose of 1 kg active substance per hectare)

NOEC<sub>te</sub> the no observed effect concentration or dose for the selected organism, (mg d<sup>-1</sup> kg<sup>-1</sup>)

The NOEC is the daily average chemical intake per kg body weight over the experimental test period. Again, an assessment factor might be introduced via adjusted toxicity data.



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## Appendix 1 Glossary

**Ctgb** board for the authorisation of plant protection products and biocides in the Netherlands. College voor de toelating van gewasbeschermingsmiddelen en biociden.

**Degradation product** Transformation product of a substance.

**DegT<sub>50</sub>** Time required for diminishing the concentration by 50% by transformation processes.

**DT<sub>50</sub>** Time required for diminishing the concentration by 50% by dissipation processes.

**EC<sub>50</sub>** 50% effect concentration, concentration at which a 50% effect is observed.

**ECC** Environmental Concern Concentration, concentration above which (eco)toxicological impacts are to be expected.

**EIU** Environmental Indicator Unit, unit to express the potential environmental impact.

**GAP** Good Agricultural Practice.

**Groundwater** Water below the groundwater level; the level at which water pressure is zero (in comparison with air pressure). In the evaluation process, the concentration of a pesticide in groundwater is the target quantity.

**K<sub>om</sub>** Equilibrium constant for the sorption of a substance on organic matter.

**LC<sub>50</sub>** Lethal concentration 50%, concentration at which 50% of the test organisms die.

**LD<sub>50</sub>** Lethal dose 50%, dose at which 50% of the test organisms die.

**LOTV** Lozingenbesluit Open Teelten en Veehouderij, regulation a.o. to reduce drift deposition on surface waters.

**Metabolite** Transformation product of a substance. In strict sense, a metabolite is a transformation product resulting from metabolic transformation of a substance; here the term is used in a broader sense indicating products from any transformation reaction, so including abiotic processes.

**MIP** Milieu-Indicator Punt. Unit for potential environmental impact, see also EIU.

**NMI** Nationale Milieu-Indicator Name (in Dutch) of the software package described in this report.

**NoEC** No (observed) Effect Concentration, concentration below which effects on organisms were not observed.

**Parent substance** Synonym for substance.

**PEARL** Pesticide Emission Assessment at Regional and Local scales. Software package used to simulate leaching of substances in the soil.

**PEC** Predicted Environmental Concentration.

**PIEC** Predicted Initial Environmental Concentration.

**PPP** Plant Protection Product. In this text PPP is used for the substance for which the possible registration is assessed.

**Substance** Term used to indicate the substance under investigation; the word is used to indicate the active ingredient of a PPP or any metabolite.

**Transformation product** Substance that is formed out of a substance by means of any biotic or abiotic reaction process.



## Appendix 2 List of symbols

$\%_{\text{drift,sw}}$	drift as influenced by application technique and drift reducing measures, (%)
$\Delta H_{\text{vap}}$	molar enthalpy of vaporisation, ( $\text{J mol}^{-1}$ ), (default value $95000 \text{ J mol}^{-1}$ )
$\Delta H_{\text{T}}$	molar enthalpy of transformation, ( $\text{J mol}^{-1}$ ), (default value $54000 \text{ J mol}^{-1}$ )
$A$	nominal rate for a single application, ( $\text{kg ha}^{-1}$ )
AE	assimilation efficiency, dependent on the species, (%)
BW	body weight of the animal, (g)
$C_{\text{PEARL}}$	concentration obtained via interpolation in the PEARL metamodel, ( $\mu\text{g dm}^{-3}$ )
$CV_{\text{crop}}$	cumulative volatilisation (% of amount reaching the crop)
$CV_{\text{soil}}$	cumulative volatilisation from the soil surface (% of amount reaching the soil)
DCI	daily chemical intake, ( $\text{mg d}^{-1}$ )
$DCI_{\text{tot,a}}$	the acute total daily chemical intake, ( $\text{mg d}^{-1}$ )
$DCI_{\text{tot,c}}$	the chronic total daily chemical intake, ( $\text{mg d}^{-1}$ )
DEE	daily energy expenditure, ( $\text{kJ d}^{-1}$ )
$\text{DegT}_{50}$	nominal half-life of the substance as listed in the substance table, (d)
$\text{DegT}_{50,l}$	local half-life in the grid cell, (d)
$d_{\text{soil}}$	the depth (thickness) of the soil layer, (m)
$d_{\text{sw}}$	depth of the surface water
$E_{\text{app,air}}$	emission to air during application, ( $\text{kg ha}^{-1}$ )
$EC_{50,s}$	50% effect concentration for soil organism(s) under reference conditions, ( $\text{mg kg}^{-1}$ )
ECC	environmental concern concentration, (e.g. $\text{mg kg}^{-1}$ or $\mu\text{g dm}^{-3}$ )
ECC <sub>gw</sub>	environmental concern concentration for a substance in groundwater, ( $\mu\text{g dm}^{-3}$ )
ECC <sub>soil,a</sub>	acute environmental concern concentration for the soil, ( $\text{mg kg}^{-1}$ )
ECC <sub>soil,c</sub>	chronic environmental concern concentration for the soil, ( $\text{mg kg}^{-1}$ )
ECC <sub>sw,a</sub>	environmental concern concentration for surface water, acute, ( $\text{mg dm}^{-3}$ )
ECC <sub>sw,c</sub>	environmental concern concentration for surface water, chronic, ( $\text{mg dm}^{-3}$ )
$E_{\text{crop,air}}$	total amount volatilised from the crop, ( $\text{kg ha}^{-1}$ )
$E_{\text{dgw}}$	emission to deeper groundwater as a result of leaching, ( $\text{kg ha}^{-1}$ )
$E_{\text{gw}}$	predicted amount leaching to groundwater (depth one metre), ( $\text{kg ha}^{-1}$ )
EIU	environmental indicator unit, (-)
$EIU_{\text{gw}}$	environmental indicator units for groundwater, (-)
$EIU_{\text{soil,a}}$	environmental indicator units for soil for the acute situation, (-)
$EIU_{\text{soil,c}}$	environmental indicator units for soil for the chronic situation, (-)
$EIU_{\text{sw,a}}$	environmental indicator units for surface water, acute, (-)
$EIU_{\text{sw,c}}$	environmental indicator units for surface water, chronic, (-)
$EIU_{\text{te,a}}$	environmental indicator units for the terrestrial ecosystem, acute, (-)
$EIU_{\text{te,c}}$	environmental indicator units for the terrestrial ecosystem, chronic, (-)
$E_{\text{soil,air}}$	total amount volatilised from soil, ( $\text{kg ha}^{-1}$ )
$E_{\text{sw,d}}$	emission to surface water by the drift process, ( $\text{kg ha}^{-1}$ )
F	fraction of food type I in diet
$f_{\text{al}}$	fraction lost by volatilisation during application, (-)
$f_{\text{AV}}$	avoidance factor, (-), (1= no avoidance, 0 = complete avoidance)

$f_d$	fraction lost by spray drift to surroundings of the treated field, (-)
$f_{d,sw}$	fraction drift to surface water, (-)
$f_{DC,crop}$	fraction of substance dissociated on crop leaves, (-)
$f_{DL}$	factor accounting for ditch length, depending on map information, (-)
$f_{dr}$	fraction lateral drainage, (-)
FE	food energy, (kJ per dry gram food)
$f_{le}$	factor to account for the fraction leaching error, (-)
$f_i$	fraction intercepted by the crop, (-)
$f_{ND}$	fraction of substance not dissociated
$f_{p,m}$	molar fraction of a parent molecule converted to the metabolite, (-)
$F_{PEARL}$	leaching fraction obtained from the PEARL metamodel, (-)
$FP_{gas}$	fraction of substance in the gas phase, (-)
$f_{sw,T}$	factor for the influence of the temperature of the surface water body, (-)
$f_T$	factor denoting the influence of temperature, (-)
$f_{TWA}$	time weighted average fraction (default is no degradation for acute exposure and 0.53 for long)
$f_v$	fraction lost by volatilisation from the soil surface, (-)
$f_w$	fraction wash-off from the crop canopy, (-, default 0)
$f_w$	factor accounting for wind direction, (-, default 0.5)
G	the content of the substance in the soil, ( $\text{kg kg}^{-1}$ )
i	food type
k	first order rate coefficient for transformation in soil, ( $\text{d}^{-1}$ )
$K_g$	transport coefficient in the gas phase, ( $200 \text{ m d}^{-1}$ )
$K_H$	Henry coefficient, (-)
$K_l$	transport coefficient in the water phase, ( $2 \text{ m d}^{-1}$ )
$K_{lg}$	liquid to gas partitioning coefficient, (-)
$K_{om}$	sorption constant from the substance table, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$K_{om,com}$	the combined sorption constant, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$K_{om,l}$	local sorption constant, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$K_{sl}$	soil to liquid partitioning coefficient, ( $\text{dm}^3 \text{ kg}^{-1}$ )
$k_{sw}$	first order rate coefficient for dissipation from surface water, ( $\text{d}^{-1}$ )
$k_{vol}$	volatilisation rate coefficient, ( $\text{d}^{-1}$ )
$LD_{50,te}$	lethal dose 50% for the selected organism, ( $\text{mg kg}^{-1}$ )
$L_{sw}$	length of the surface water (per ha field), (m)
M	molar mass, ( $\text{g mol}^{-1}$ )
MC	moisture content of the food, (%)
$ME_{tot}$	the total metabolisable energy, (kJ)
$NOEC_s$	no observed effect concentration for soil organism, ( $\text{mg kg}^{-1}$ )
$NOEC_{te}$	the no observed effect concentration or dose for the selected organism, ( $\text{mg kg}^{-1}$ )
$OM\%_{gridcell}$	organic matter of the grid cell soil, (percentage)
$OM\%_{ref}$	organic matter of the (reference) test medium, (%)
$om_s$	the local organic matter fraction in the topsoil (upper 5 cm), (-)
$om_{grid}$	organic matter content in the top 35 cm layer of the grid cell, (%)
$om_{ref}$	organic matter content in the top layer of the reference, (%)
PEC	predicted environmental concentration, (e.g. $\text{mg kg}^{-1}$ or $\mu\text{g dm}^{-3}$ )

$PEC_{gw}$	predicted environmental concentration in groundwater, ( $\mu\text{g dm}^{-3}$ )
$pH_{app}$	pH of the application solution, (-)
$PIEC_{soil}$	predicted initial environmental concentration in soil, ( $\text{mg kg}^{-1}$ )
$PIEC_{sw}$	initial concentration in surface water immediately after application, ( $\text{mg dm}^{-3}$ )
$P_{sat}$	saturated vapour pressure of the substance (mPa)
$P_{sat,r}$	saturated vapour pressure of the substance (mPa) under reference conditions
$R$	molar gas constant, ( $\text{J mol}^{-1} \text{K}^{-1}$ )
$RUD$	residue unit dose, (mg per kg fresh weight food per unit dose of 1 kg $\text{ha}^{-1}$ )
$S_N$	net soil deposition, ( $\text{kg ha}^{-1}$ )
$S_{N,T}$	total net soil load, ( $\text{kg ha}^{-1}$ )
$S_{sw}$	net surface water deposition, ( $\text{kg ha}^{-1}$ (surface water))
$S_{sw,r}$	the amount in surface water immediately before the last application, ( $\text{kg ha}^{-1}$ ), the remains of former applications
$S_{sw,t}$	the amount in surface water at time $t$ (= time after last application), ( $\text{kg ha}^{-1}$ )
$S_{sw.ta}$	the amount in surface water immediately after the last application, ( $\text{kg ha}^{-1}$ )
$t$	time (= time elapsed after last application), (d)
$t_{exp}$	appropriate exposure time, (d)
$T_{gridcell}$	average monthly temperature of the grid cell, (K)
$T_{gridcell,lt}$	long term average temperature of the grid cell, (K)
$T_r$	reference temperature, (K), (value 293.15 K $\equiv 20^\circ\text{C}$ )
$T_{SS}$	long term average temperature of reference scenario, (K)
$TWA_{soil}$	time weighted average environmental concentration in soil, ( $\text{mg kg}^{-1}$ )
$V_{sw}$	volume of water per m length of standard ditch, ( $0.21 \text{ m}^2$ )
$W_{sw}$	width of the surface water (wet surface), (m)
$X_R$	content in soil immediately before the last application, ( $\text{kg kg}^{-1}$ )
$X_t$	content in soil at time $t$ , ( $\text{kg kg}^{-1}$ )
$X_{TA}$	content in soil immediately after the last application, ( $\text{kg kg}^{-1}$ )
$\alpha$	acute angle of the slope of the ditch with the soil surface
$\varepsilon_{gas}$	volumetric gas fraction, (volume gas per volume soil)
$\varepsilon_{liquid}$	volumetric liquid fraction, (volume soil solution per volume soil)
$\rho_{soil}$	soil dry bulk density, ( $\text{kg dm}^{-3}$ )



## Appendix 3 Crops included in NMI version 2

Table A3.1 Crops, sectors and total areas represented in the NMI, data are for 1998 and for 2004

Crop	Sector	Area (ha)	
		1998	2004
winter wheat	akkerbouw (arable farming)	127673	117121
sugar beets		112551	97392
ware potatoes		84023	72543
starch potatoes		56936	51490
seed potatoes		39889	39706
spring barley		36528	44683
grass (seed)		28418	25327
onions		13844	19889
peas		4589	4862
onions (bulbs)		4505	5604
chicory		4196	4918
haricot beans		2381	2658
field beans		1690	-
summer wheat		-	20822
flax		-	4461
tulips	bloembollenteelt (flowerbulb cultivation)	9847	10873
lilies		3609	4358
daffodils		1572	1773
gladiolas		1360	1275
hyacinths		1181	1137
iris		664	554
roses (glasshouse)	bloemisterij glas (glasshouse floristry)	931	848
chrysanthemum		757	679
pot plants (flowers)		636	767
pot plants (green)		540	573
bedding plants		449	543
freesias		241	191
lilies (glasshouse)		237	273
gerberas		219	227
orchids		206	233
carnation		117	-
alstroemeria		-	85
tree nursery	boomkwekerij (cultivation of trees)	2955	3593
floriculture		2432	2407
shrubberies		2277	2301
conifers		1822	2734
fruit trees		1304	1146
perennial plants		947	1389
roses		716	463

Table A3.1 continued

Crop	Sector	Area (ha)	
		1998	2004
mushrooms	eetbare paddestoelen (mushrooms)	98	84
apple trees		14679	10212
pear trees	fruitteelt (fruit cultivation)	5938	6495
tomatoes	groenteteelt glas (greenhouse vegetables)	1305	1352
sweet pepper		1010	1206
cucumbers		710	623
radish		-	109
green beans	groenteteelt vollegrond (open air vegetables)	4852	4405
carrots (winter)		4822	5453
Brussels sprouts		4622	3455
industrial chicory roots		4242	2938
leeks		3641	3039
cabbage		2940	2574
carrots		2934	2436
asparagus		2304	2362
strawberries		1967	2129
salsify		1839	1020
cauliflower		-	2322
grass	veehouderij (cattle farming)	1031771	983386
fodder maize		239288	224368

## Appendix 4 Crop interception fractions

Table A4.1 Crop interception fractions for spraying applications to field crops<sup>1</sup>

crop	sector	mode of action	application time (month number)												
			1	2	3	4	5	6	7	8	9	10	11	12	
onions (bulbs)	arable farming		-	-	-	0.145	0.166	0.428	0.457	0.171	-	-	-	-	
onions			-	-	0.116	0.166	0.166	0.428	0.457	0.457	0.137	-	-	-	
peas			0.013	0.013	0.065	0.187	0.383	0.709	0.720	0.307	0.013	0.013	0.013	0.013	
field beans			-	-	-	-	0.175	0.750	0.900	0.788	-	-	-	-	
seed potatoes			0.002	0.002	0.002	0.060	0.315	0.632	0.843	0.780	0.002	0.002	0.002	0.002	
haricot beans			-	-	-	-	0.075	0.500	0.800	0.863	0.630	-	-	-	
starch potatoes, ware potatoes			0.002	0.002	0.002	0.019	0.162	0.459	0.688	0.891	0.750	0.088	0.002	0.002	
sugar beets			0.013	0.013	0.013	0.078	0.187	0.239	0.415	0.796	0.796	0.502	0.013	0.013	
flax, spring barley, summer wheat			-	-	0.014	0.377	0.855	0.868	0.824	0.309	-	-	-	-	
chicory			-	-	-	0.075	0.200	0.260	0.463	0.900	0.900	0.563	-	-	
winter wheat			0.047	0.047	0.164	0.398	0.856	0.868	0.824	0.823	0.247	-	0.018	0.047	
grass (seed)			0.250	0.250	0.250	0.250	0.469	0.740	0.900	0.900	0.900	0.331	0.250	0.250	
daffodils, hyacinths, tulips	flowerbulb cultivation		-	-	0.183	0.262	0.357	0.492	-	-	-	-	-	-	
gladiolas			-	-	-	-	0.044	0.500	0.363	0.329	0.308	0.039	-	-	
lilies			-	-	-	-	0.060	0.498	0.364	0.328	0.307	0.038	-	-	
iris			-	-	0.183	0.262	0.357	0.548	0.568	0.213	-	-	-	-	
floriculture	cultivation of trees	herb.	-	-	0.183	0.262	0.357	0.492	-	-	-	-	-	-	
		fung., insect.	0.100	0.100	0.100	0.100	0.264	0.290	0.290	0.290	0.290	0.290	0.290	0.106	0.100
tree nursery		herb.	0.080	0.080	0.080	0.080	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.080	

fruit trees		fung., insect.	0.120	0.120	0.120	0.120	0.383	0.420	0.420	0.420	0.420	0.420	0.308	0.120
		herb.	0.118	0.118	0.118	0.118	0.354	0.388	0.388	0.388	0.388	0.388	0.287	0.118
roses		fung., insect.	0.010	0.010	0.010	0.026	0.164	0.467	0.700	0.907	0.764	0.702	0.089	0.010
		herb.	-	-	-	0.018	0.157	0.429	0.640	0.826	0.697	0.641	0.088	-
shrubberries		fung., insect.	0.010	0.010	0.010	0.026	0.164	0.467	0.700	0.907	0.764	0.702	0.439	0.010
		herb.	-	-	-	0.018	0.157	0.429	0.640	0.826	0.697	0.641	0.404	-
perennial plants		fung., insect.	0.010	0.010	0.010	0.613	0.700	0.700	0.700	0.700	0.700	0.700	0.438	0.010
		herb.	-	-	-	0.561	0.640	0.640	0.640	0.640	0.640	0.640	0.404	-
conifers		fung., insect.	0.560	0.560	0.560	0.560	0.560	0.560	0.560	0.560	0.560	0.560	0.560	0.560
		herb.	0.514	0.514	0.514	0.514	0.514	0.514	0.514	0.514	0.514	0.514	0.514	0.514
apple trees, pear trees	fruit cultivation	fung., insect.	0.120	0.120	0.120	0.120	0.453	0.636	0.740	0.665	0.620	0.620	0.433	0.120
		herb.	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100	0.100
leeks	open air vegetables		0.009	0.009	0.009	0.009	0.009	0.084	0.159	0.325	0.424	0.268	0.009	0.009
green beans			-	-	-	-	-	0.100	0.575	0.863	0.270	-	-	-
salsify			-	-	-	-	-	0.082	0.199	0.454	0.454	0.454	0.283	-
asparagus			-	-	-	-	-	0.100	0.238	0.500	0.500	0.500	0.313	-
strawberries			0.234	0.234	0.234	0.234	0.351	0.335	0.058	0.234	0.234	0.234	0.234	0.234
Brussels sprouts, cabbage, cauliflower			-	-	-	-	-	0.210	0.538	0.800	0.800	0.800	0.500	-
carrots (winter)			0.006	0.006	0.006	0.006	0.077	0.250	0.770	0.852	0.852	0.852	0.535	0.006
carrots, industrial chicory roots			-	-	-	-	0.075	0.260	0.813	0.900	0.900	0.900	0.563	-
fodder maize	(cattle farming)		0.001	0.001	0.001	0.001	0.038	0.219	0.620	0.787	0.843	0.527	0.001	0.001
grass			0.050	0.050	0.169	0.411	0.794	0.900	0.900	0.900	0.900	0.120	0.020	0.023

1 in case of soil treatment (surface applications), the crop interception factor is 0.1 for all crops and application times.

## Appendix 5 NMI database input for substances

**Table A5.1 Substance input data to be provided by the user and stored in the NMI database**

<b>Physico-chemical properties</b>		<b>units</b>
Psat	saturated vapour pressure	mPa
M	molar mass	g mol <sup>-1</sup>
S	solubility	mg dm <sup>-3</sup>
DegT <sub>50,s</sub>	half life in soil	d
DegT <sub>50,sw</sub>	half life in soil/water systems	d
K <sub>OM</sub>	sorption constant	dm <sup>3</sup> kg <sup>-1</sup>
K <sub>OM,base</sub>	sorption constant, base	dm <sup>3</sup> kg <sup>-1</sup>
K <sub>OM,acid</sub>	sorption constant, acid	dm <sup>3</sup> kg <sup>-1</sup>
pK <sub>a</sub>	dissociation constant	-
f <sub>fle</sub>	factor for correcting leaching emissions and concentrations	-
f <sub>p,m</sub>	the molar fraction of a parent molecule converted to the metabolite	-
<b>Toxicity values</b>		
EC <sub>50,s</sub>	acute toxicity value for soil organisms (EC <sub>50</sub> or LC <sub>50</sub> )	mg kg <sup>-1</sup>
NOEC <sub>s</sub>	chronic toxicity value for soil organisms	mg kg <sup>-1</sup>
EC <sub>50,sw</sub>	acute toxicity value for aquatic organisms (EC <sub>50</sub> or LC <sub>50</sub> ) or for the aquatic ecosystem	mg dm <sup>-3</sup>
NOEC <sub>sw</sub>	Chronic toxicity value for aquatic organisms (NOEC) or for the aquatic ecosystem	mg dm <sup>-3</sup>
LD <sub>50,te</sub>	acute toxicity value for the terrestrial organism	mg kg <sup>-1</sup>
NOEC <sub>te</sub>	chronic toxicity value for the terrestrial organism	mg kg <sup>-1</sup>
t <sub>exp</sub>	exposure time (duration of the experiment; used for determining chronic effect value; the data have to be provided for both soil and the surface water compartment)	d
ECC <sub>gw</sub>	environmental concern concentration for groundwater; usually the threshold value for drinking water is taken	µg dm <sup>-3</sup>
<b>Miscellaneous</b>		
substance name (Dutch)		-
substance name (English)		-
substance number (RAB)		-
spraying application class code		-
substance group (fungicide, insecticide, herbicide, other)		-
CAS number.		-



## Appendix 6 Input parameters for terrestrial ecosystem

Table A6. 1 Default input parameters for calculating the exposure of birds and mammals

	fraction of diet	FE kJ/g dw	MC %	AE %@	AE %#	RUD (fw) <sup>\$</sup>	RUD (fw) <sup>&amp;</sup>	f <sub>AV</sub>
short grass	0.22	18	76.4	46	37.2	61.6	142	1
long grass	0	18	76.4	46	37.2	21.3	69	1
leaves	0.21	11.2	88.6	74	76	25	87	1
leafy crops	0	11.2	88.6	74	76	25	87	1
forage crops	0	18	82.1	74	76	25	87	1
small seeds	0.385	21	11.9	83	78.7	25	87	1
fruit	0	11.6	83.7	74	55.8	2.3	11	1
pods	0	21	11.9	83	78.7	2.3	11	1
large seeds	0.065	16.7	13.3	83	78.7	2.3	11	1
small insects (foliar appl.)	0.12	21.9	70.5	88	72	25	87	1
large insects (foliar appl.)	0	21.9	70.5	88	72	2.7	11	1
insects (soil applications)	0	21.9	70.5	88	72	0.1	1	1

@ mammals

# birds

\$ long term exposure

& acute exposure

**RIVM**

National Institute  
for Public Health  
and the Environment

P.O. Box 1  
3720 BA Bilthoven  
The Netherlands  
[www.rivm.com](http://www.rivm.com)