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J.J.T.I. Boesten[1], M.C. Braakhekke[1], E.L. Wipfler[1], E.A. van Os[2], M.J.J. Hoogsteen[3]

1 Wageningen Environmental Research WUR
2 WUR Greenhouse Horticulture
3 National Institute for Public Health and the Environment

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Experiences with previous versions of the Greenhouse Emission Model (GEM) for soilless cultures prompted the need for developing a revised version. GEM consists of a submodel for the water flows in the greenhouse (the WaterStreams Model, WSM) and a submodel for the pesticide behaviour in the greenhouse (the Substance Emission Model, SEM). The resulting emission fluxes are used by the TOXSWA model to simulate concentrations in surface water. This report describes the changes in WSM and provides a full description of the concepts and equations in the revised SEM version The main changes in WSM are the extension of options: (i) emission norms for nitrogen up to 2027 can be used, (ii) sodium levels can be set by the user, (iii) options for managing the discharge to the surface water are extended, (iv) a waiting time can be prescribed between a pesticide application and the next discharge. Option (ii) and (iv) are only available is used as a standalone model, i.e. outside GEM. There are two types of SEM: SEM-S for crops grown on slabs and SEM-P for crops grown in pots on tables. Main changes in SEM-S include: (i) the water in the slabs is divided into two equal parts with root uptake restricted to the first part, (ii) sorption to the slab material and the irrigation pipes is included, (iii) the amounts present in the air and condensation water immediately after spray or Low Volume Mister (LVM) application are strongly reduced, (iv) for spray and LVM applications direct contamination of the slabs, the drainage-water troughs, and the roof is added. Main changes in SEM-P include: (i) the amounts present in the air and condensation water immediately after an application are strongly reduced, (ii) the sorption equilibrium between the bottom 10 cm of the pots and the water on the tables was removed, (iii) for spray of LVM applications, the deposition on the tables is increased from about 10 to about 40%.

Keywords: soilless cultures, pesticides, emissions to surface water, greenhouse cultivation, greenhouse model

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Approved team leader responsible for the contents,

name: Maikel de Potter

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Preface

The Greenhouse Emission Model (GEM) has been developed to estimate the emission of pesticides from soilless grown greenhouse crops via the water emission route to surface water. In the past years, experience was gained with this model for regulatory use, GEM was tested and the process descriptions were reviewed, which generated a number of proposals to improve model concepts.

This report describes the process descriptions of the revised GEM model for soilless cultivations which were implemented in the new version of GEM. Suggestions for substance properties to be used in the assessment will become part of the user manual of GEM4.

Summary

Introduction

The Greenhouse Emission Model (GEM) has been developed as a tool to estimate the emission of pesticides from soilless grown greenhouse crops via the water emission route to surface water. Emissions are estimated based on the latest insights in Dutch grower practices. A first description of GEM was published by Van der Linden et al. (2015). Based on further analysis and experiences gained with the GEM3.2.2 model in the context of the environmental risk assessment of pesticides, a new version has been developed of which the concepts are described in this report.

Crops in soilless cultivations are generally grown in (stonewool) slabs or in pots. These pots are then irrigated via a so-called eb and flood system. For both types of growing systems the excess of irrigation water is collected in troughs and this collected water is reused for irrigation (reuse of irrigation water is obligatory in the Netherlands). Also, condensation water from the greenhouse roof is collected and reused as irrigation water. Before reuse the water is filtered and disinfected to remove possible pathogens. Pesticide is applied via the nutrient solution, via spraying or with a low volume mister. Discharge of recirculation water to surface water occurs mainly due to exceedance of the sodium concentration thresholds but also filter cleaning water is discharged. Pesticide enters the recirculation water through direct application in the mixing tank, deposition on slabs, tables or on the troughs or via the collected condensation water. Discharge of recirculation water hence leads to emission of pesticides to nearby surface waters. The discharged water is treated before being released with an obligatory minimum removal rate of 95%.

GEM consists of three underlying sub-models: there is one sub-model for simulating the water flows in the greenhouse (the WaterStreams Model, WSM) and a second sub-model for the pesticide behaviour in the greenhouse (the Substance Emission Model, SEM). The resulting emission fluxes are used by third model (the TOXSWA model) to simulate concentrations in surface water. Improvements were done in the WaterStreams model and the Substance Emission Model only. The parameterisation of the TOXSWA model remained unchanged.

The WaterStreams model (WSM)

The WaterStreams Model estimates the ingoing and outgoing water flows at a commercial nursery. The model uses a crop transpiration model to simulate the water uptake for crop growth, using daily meteorological data are used as input. All soilless grown greenhouse crops are mapped to four representative crops: tomato, sweet pepper, rose and ficus. These crops were selected based on their tolerance to higher sodium levels and their water uptake. The WSM calculates for each of these representative crops and per hour the amount of used rainwater, possible additional external water used (e.g tapwater or osmosis water) and the volume of condensation water. Further, the crop uptake, the required amount of discharge of the nutrient solution (resulting from Na^+ accumulation above the threshold value), the required filter cleaning water and emissions of nitrogen are calculated, while simulating typical grower management practices. The main changes in WSM relevant to GEM are the extension of options: (i) emission norms for nitrogen up to 2027 have been implemented and can be selected by the user, (ii) options for managing the discharge to the surface water from filter cleaning water.

The substance emission model (SEM)

Based on the in- and outgoing waterflows provided by WSM, SEM describes the water flows inside the greenhouse and between a series of tanks that represent the water in the slabs and the various tanks through which the recirculation water flows. The water in one of these tanks (the wastewater tank) is emitted to the surface water; the concentrations in this emission water may be multiplied with a reduction factor to account for the obligatory purification of the water. SEM can be used for applications via the drip irrigation water, spray applications, and LVM applications. For application via drip irrigation the applied dose is added directly to the recirculation water (in the mixing tank). For

spray application and LVM, the applied dose enters the recirculation water via direct deposition on slabs, tables or on the troughs or via the collected condensation water.

The substance emission model for crops grown on slabs (SEM-S)

For crops grown in slabs, SEM has been revised based on an earlier review of the process descriptions. The main changes include:

1. sorption to the slab material (e.g. stonewool), foil covering the slabs, and the walls of the irrigation pipes has been added, as well as partitioning into the roots (leading to decreased emission concentrations),
2. the amounts of pesticide in the air plus condensation water immediately after a spray or LVM application have been strongly reduced (from 8% to 0% for spray and from 35% to about <1% for LVM applications, leading to decreased emission concentrations),
3. the concentration in the air at the plant surface has been reduced from 100% to 20% of the saturated vapour concentration (leading to decreased emission concentrations),
4. in case of spray or LVM applications, small parts of the dose (0.1-1%) are now directly deposited during application on the slabs, the troughs that collect the drainage water of the slabs, and (c) the roof. In the former version of the model there was not direct deposition (leading to increased emission concentrations),
5. after spray or LVM applications, about 40% of the dose is deposited onto the plants and about 60% on the floor compared to 55-80% on the plants and 10-20% on the floor in the previous version. For LVM first the air is saturated and the remaining applied dose is deposited (leading to increased emission concentrations).

A further main change considers the cultivation tank which represents the water in the slabs. This tank is now subdivided into two parts with equal volume, while uptake of water and pesticide by the roots of the crop is restricted to the first part. This change was based on a previous test for application by drip irrigation to stonewool slabs. The change leads to decreased emission concentrations.

The implementations of spraying or LVM as pesticide application method are very similar, but not the same. Differences between spray and LVM applications in SEM-S are:

- for spray applications, the air is free of pesticide immediately after application, whereas it is saturated with pesticide immediately after an LVM application,
- the fraction deposited on the roof is 1% after spray applications and 0.1% after LVM applications,
- volatilisation from plants proceeds faster after spray applications because spraying leads to deposition of droplets onto both sides of the leaves whereas LVM applications generate only droplets on the upper side of the leaves.

The substance emission model for crops grown in pots in an ebb/flood system on tables or floors (SEM-P)

For crops grown in pots, SEM has been revised based on an earlier review of the process descriptions in SEM-P. The main changes in the model are:

1. the amounts of pesticide in the air plus the condensation water immediately after a spray or LVM application have been strongly reduced (leading to decreased emission concentrations),
2. the concentration in the air at the plant surface after spray or LVM applications has been reduced from 100% to 20% of the saturated vapour concentration (leading to decreased emission concentrations),
3. explicit simulation of sorption of pesticide in the water on the tables to organic matter in the bottom 10 cm of the pots has been removed (leading to increased emission concentrations),
4. exchange between the water on the tables and the air (via volatilisation or deposition) has been removed (leading to increased emission concentrations),
5. it is assumed that spray or LVM applications occur when tables are dry. Deposited pesticide can volatilize from the tables until 1 d after application, when the remaining deposit is dissolved in the irrigation water, i.e. the tables are flooded after one day (leading to decreased emission concentrations),
6. for spray or LVM applications, deposition of 0.1-1% of the dose on the roof has been added (leading to increased emission concentrations),

7. for spray or LVM applications, about 40% of the dose is deposited on the tables, about 20% on the pots and about 40% on the plants compared to about 7-8% on tables, 3-4% on pots and 55-80% on plants in the previous version. For LVM, first the air is saturated and the remaining applied dose is deposited (leading to increased emission concentrations because of the increased deposition on the tables),
8. the submodel of the pots that describes the behaviour of the pesticide deposited on the pot surface includes also diffusion in liquid phase and a deeper penetration into the pot (a priori unknown effect on emission concentrations). Note that sorption is considered for the substance deposited on the pots (not on the tables, see point (3)).

Differences between spray or LVM applications for pots are the same as for slabs (see bullet list above).

Samenvatting

Inleiding

Het Greenhouse Emission Model (GEM) berekent de emissie van gewasbeschermingsmiddelen naar het oppervlaktewater vanuit kasteelten (substraatteelt, teelt boven de grond). Daarbij wordt uitgegaan van de Nederlandse kasteeltpraktijk. De blootstellingscenario’s en modelconcepten van GEM (versie 3.2.2) zijn beschreven in Van der Linden et al. (2015). Het GEM3.2.2 model wordt op dit moment gebruikt bij de milieurisicobeoordeling van gewasbeschermingsmiddelen in Nederland. Nieuwe wetenschappelijke inzichten en ook ervaringen opgedaan met GEM in de toelating zijn aanleiding geweest voor een aantal verbeteringen van het GEM model. Deze zijn beschreven in dit rapport. Door deze verbeteringen is het model beter in staat concentraties in het oppervlaktewater te berekenen als gevolg van gebruik van gewasbeschermingsmiddelen in gangbare Nederlandse substraatteelten.

Onder substraatteelten worden de ‘boven de grond’ teelten beschouwd in bijvoorbeeld steenwol matten en in potten (met bijv. potgrond of kokos). Water en voedingsstoffen (gietwater) worden toegediend via druppel-bevloeiing of via een eb- en vloedsysteem. Het teveel aan gietwater wordt vervolgens opgevangen, gezuiverd en ontsmet voor hergebruik. Het gezuiverde en ontsmette water wordt ook wel recirculatiewater genoemd. Het condenswater dat zich vormt op het dak van de kas wordt opgevangen en toegevoegd aan het recirculatiewater. De gewasbeschermingsmiddelen worden toegepast via een druppelbehandeling/ met de voedingsoplossing of door gewasbespuitingen. Ook vinden er ruimtebehandelingen plaats met behulp van zogenaamde Low Volume Misters (LVM). Het recirculatiewater wordt geloosd om het natriumgehalte in het giftwater te beheersen. Ook wordt er recirculatiewater geloosd als gevolg van het schoonspoelen van het filter. Gewasbeschermingsmiddelen vinden hun weg naar het recirculatiewater door directe toediening aan het recirculatiewater in het meng reservoir, door depositie (bij spuittoepassing) op de matten, tafels en drainagebakken of via het opgevangen condenswater. De lozing van recirculatiewater kan dus leiden tot emissie van gewasbeschermingsmiddelen naar het oppervlaktewater. Sinds enkele jaren is het verplicht om het geloosde water te zuiveren met een minimale verwijderingspercentage van 95 procent.

GEM maakt gebruik van drie onderliggende sub-modellen. Het eerste sub-model simuleert de waterstromen in de kas (het ‘WaterStreams model’) en het tweede sub-model simuleert het gedrag van gewasbeschermingsmiddelen in de kas (het ‘Substance Emission Model’, SEM). De lozing van water en middel dat wordt berekenend door WaterStreams en SEM is invoer voor het derde sub-model: TOXSWA. Dit model berekent de concentraties in het ontvangende oppervlaktewater. De verbeteringen die zijn doorgevoerd in GEM vonden plaats aan het WaterStreams model en het SEM model. Het TOXSWA model is gelijk gebleven.

Het WaterStreams model (WSM)

Het WaterStreams model (WSM) berekent de in- en uitgaande waterstroming voor kasteelten. De waterbehoefte van het gewas wordt berekend met behulp van een gewasverdampingsmodel op basis van specifieke gewaseigenschappen en weergegevens. Voor het berekenen van de dagelijkse lozingen zijn er vier representatieve gewassen geselecteerd: tomaat, paprika, roos en ficus. Elk van deze gewassen representeert een andere combinatie van zouttolerantie en waterbehoefte. WSM berekent voor de representatieve gewassen de inname van regenwater (vanuit het opvangbassin), eventuele additionele waterbronnen (bijv. leidingwater) en het volume condenswater dat wordt opgevangen en toegevoegd aan het recirculatiewater. Ook wordt de wateropname van het gewas berekend en het watervolume dat wordt geloosd op het oppervlaktewater als gevolg van een te hoog zoutgehalte of van het doorspoelen van het filter. De belangrijkste uitbreidingen die zijn doorgevoerd aan het WSM model, welke tevens zijn opgenomen in GEM4, zijn: (i) emissienormen voor de emissie van nitraat zoals vastgesteld in het Activiteitenbesluit Milieubeheer 2017 zijn doorgevoerd tot en met 2027 en kunnen worden geselecteerd door de gebruiker, (ii) optie om te kiezen voor lozen van filterspoelwater of hergebruik ervan.

Het ‘substance emission model’ (SEM)
Het stofstromenmodel SEM beschrijft het gedrag/de lotgevallen van gewasbeschermingsmiddelen in de kas. De informatie over de in- en uitgaande waterstromen van WSM wordt door SEM vertaald naar waterstromen tussen de verschillende waterreservoirs in een kas. Samen bevatten deze reservoirs het totale volume aan recirculatiewater. Het afvalwater-reservoir is één van deze reservoirs. Het water in het afvalwater reservoir wordt geloosd naar het oppervlaktewater. Een door de gebruiker in te voeren reductiefactor representeert het effect van de zuivering van het lozingswater. SEM berekent concentraties in het lozingswater voor druppel- en spuittoepassingen en ook voor ruimtebehandelingen (LVM). Bij druppeltoepassingen wordt het middel direct aan het recirculatiewater toegevoegd. Bij spuittoepassingen en LVM vindt er depositie plaats op de matten en de tafels alsook de drainage opvanggoten. Ook vindt er directe depositie plaats tegen het dak. Het middel kan dan via het condenswater in het recirculatiewater terechtkomen.

Het ‘substance emission model’ voor gewassen op matten (SEM-S)
SEM is aangepast voor gewassen op matten op de volgende wijze:

1. sorptie aan de matten, het plastic folie rond de matten, en de wanden van de irrigatiepijpen is toegevoegd aan het model. Daarnaast is uitwisseling van stoffen tussen wortels en recirculatie water (partitie) toegevoegd aan het model. Deze aanpassing leidt tot een afname van de berekende concentraties van het lozingswater;
2. het gehalte gewasbeschermingsmiddel in de lucht (plus het condenswater) direct na een spuittoepassing of een ruimtebehandeling is verlaagd. In het oude GEM model werd 8 procent aangenomen van de totale dosering. In het nieuwe model is het 0 procent bij spuittoepassingen en gelijk aan de verzadigde dampconcentratie voor ruimtebehandelingen Deze aanpassing leidt tot een afname van de berekende concentraties van het lozingswater;
3. de concentratie in de lucht net boven het bladoppervlak van het gewas is verlaagd van 100 procent naar 20 procent van de verzadigde dampconcentratie. Deze aanpassing leidt tot verlaging van de concentraties in het lozingswater;
4. bij spuittoepassingen en ruimtebehandelingen wordt gerekend met een depositie van 0.1-1 procent van de dosering op de matten, de drainage goten en het dak. Deze aanpassing leidt tot een verhoging van de concentraties in het lozingswater;
5. daarnaast wordt gerekend met 40 procent van de dosering op de planten en 60 procent op de vloer. In het oude model was dit 55-80 procent op de plant en 10-20 procent op de vloer. Let wel: voor ruimtebehandeling komt eerst een deel in de kaslucht (zie punt (2)). Deze aanpassing leidt tot een verhoging van de concentraties in het lozingswater;

Naast deze wijzigingen is er een wijziging aangebracht in de wijze waarop het teeltgedeelte van de kas (planten, matten en buizen) wordt gerepresenteerd in het model. Dit teeltgedeelte werd in GEM3.3.2 gerepresenteerd door één reservoir. Dit reservoir is in GEM4 verdeeld in twee compartimenten. Beide compartimenten gaan uit van volledige menging en eventueel afbraak van middel en sorptie aan matten en plastic, echter gewasopname en partitie tussen recirculatiewater en wortels vindt uitsluitend plaats in het eerste compartiment. Deze aanpassing is gedaan naar aanleiding van de validatietest van GEM-substraat en leidt naar verwachting tot lagere berekende concentraties in het lozingswater.

De toediening van gewasbeschermingsmiddel via spuittoepassing en ruimtebehandeling wordt op een vergelijkbare wijze gesimuleerd door SEM. Verschillen tussen de twee typen toepassingen zijn:

- bij spuittoepassingen is het gehalte gewasbeschermingsmiddel in de lucht vlak na toepassing nul en bij ruimtebehandeling gelijk aan de verzadigde concentratie;
- de depositiefractie op het dak van de kas is 1 procent voor spuittoepassingen en 0.1 procent voor ruimtebehandelingen;
- de vervluchtiging vanaf het bladoppervlak van het gewas is sneller voor spuittoepassingen omdat de druppels aan beide kanten van het blad terechtkomen, terwijl bij ruimtebehandelingen de druppels alleen aan de bovenkant terechtkomen.

Het ‘substance emission model’ voor potplanten op eb- en vloedsystemen op tafels en vloeren (SEM-P)

De belangrijkste aanpassingen aan SEM voor de simulatie van toepassingen van gewasbeschermingsmiddel in potplanten zijn:

1. het gehalte gewasbeschermingsmiddel in de lucht (plus het condenswater) direct na een spuittoepassing of een ruimtebehandeling is verlaagd op dezelfde wijze als voor de matten. Deze aanpassing leidt tot een afname van de berekende concentraties van het lozingswater;
2. de concentratie in de lucht net boven het bladoppervlak van het gewas is verlaagd van 100 procent van de verzadigde dampconcentratie naar 20 procent van de verzadigde dampconcentratie. Deze aanpassing leidt tot verlaging van de concentraties in het lozingswater;
3. sorptie aan het organisch materiaal in de potten van stoffen in het water op de tafels wordt niet meer expliciet gesimuleerd. Deze aanpassing leidt tot een verhoging van de berekende concentraties van het lozingswater;
4. De toepassing van gewasbeschermingsmiddel vindt plaats als de tafels droog zijn. Daarna vindt er vervluchtiging plaats vanuit de tafels naar de kaslucht gedurende 1 dag. Daarna wordt verondersteld dat de tafels worden gevuld met gietwater en dat het middel oplost in het gietwater. Deze aanpassing leidt tot verlaging van de concentraties in het lozingswater;
5. de uitwisseling tussen het water op de tafels en de kaslucht wordt niet meer gesimuleerd; het water staat maar kort op de tafels en verondersteld wordt dat dit proces een verwaarloosbaar effect heeft. Deze aanpassing leidt tot een verhoging van de berekende concentraties van het lozingswater;
6. bij spuittoepassingen en ruimtebehandelingen wordt gerekend met een depositie van 0.1-1 procent van de dosering op het dak. Deze aanpassing leidt tot een verhoging van de concentraties in het lozingswater;
7. daarnaast wordt gerekend met 40 procent van de dosering op de planten, 40 procent of de tafels en 20 procent potten. In het oude model was dit 55-80 procent op de plant en 3-4 procent op de potten en 7-8 procent op de tafels. Let wel: voor ruimtebehandeling komt eerst een deel in de kaslucht (zie punt (1) hierboven). Deze aanpassing leidt tot een verhoging van de concentraties in het lozingswater;
8. aan het sub-model dat het gedrag in de pot beschrijft is diffusie in water als transportproces toegevoegd en ook kan de stof dieper in de pot binnendringen na depositie. Dit sub-model simuleert overigens wel sorptie aan het organische materiaal.

Verschillen tussen spuit en ruimtebehandelingen zijn verder gelijk aan die bij matten (zie boven).

1 Introduction

1.1 Background

The Greenhouse Emission Model (GEM) is a software instrument that has been developed to estimate the emission of pesticides from greenhouse crops to surface water. The instrument allows for calculation of emissions from soilless cultivated crops and soil-bound cultivated crops.

In the past years, experience was gained with this model for regulatory use. At the same time GEM was tested twice for soilless cultivated crops, i.e. for application of pesticides to stonewool via the irrigation water (Van der Linden et al., 2017; Wipfler et al., 2020). Also, the process descriptions for soilless cultivation were reviewed (Boesten et al., 2019). All of these activities generated a number of proposals to improve model concepts. Furthermore, GEM needed to be extended to include application via the nutrient solution to crops grown in pots in an ebb/flood or sub-irrigation system. This report describes the processes of the revised GEM model for soilless cultivations. With the final aim to implement these into a new version of the GEM instrument.

1.2 Overview of the GEM modelling system

The GEM software for soilless cultivations consists of three models (Figure 1):

- the ‘WaterStreams’ model (WSM), which calculates, on a 1-h basis, (i) the water requirements of the crop per ha greenhouse based on meteorological data and the sodium concentration in the irrigation water, (ii) the volume of condensation water that is generated per ha greenhouse, (iii) the water volume that is discharged to the surface water per ha greenhouse, and (iv) the air temperature in the greenhouse;
- the substance emission model (SEM), which calculates, on an hourly basis, the emission of substances (a pesticide and possibly degradation products) to the surface water;
- the TOXSWA model, which calculates resulting concentrations of substances in the surface water.

This report describes the changes in the WaterStreams model compared with the previous release of GEM (Chapter 2) and the model concepts and parameterisation of the SEM sub-models for crops grown on slabs (Chapter 3) and crops grown in pots (Chapter 4). The concepts and parameterisation of TOXSWA are described elsewhere (Van der Linden et al., 2015; Wipfler et al., 2015).

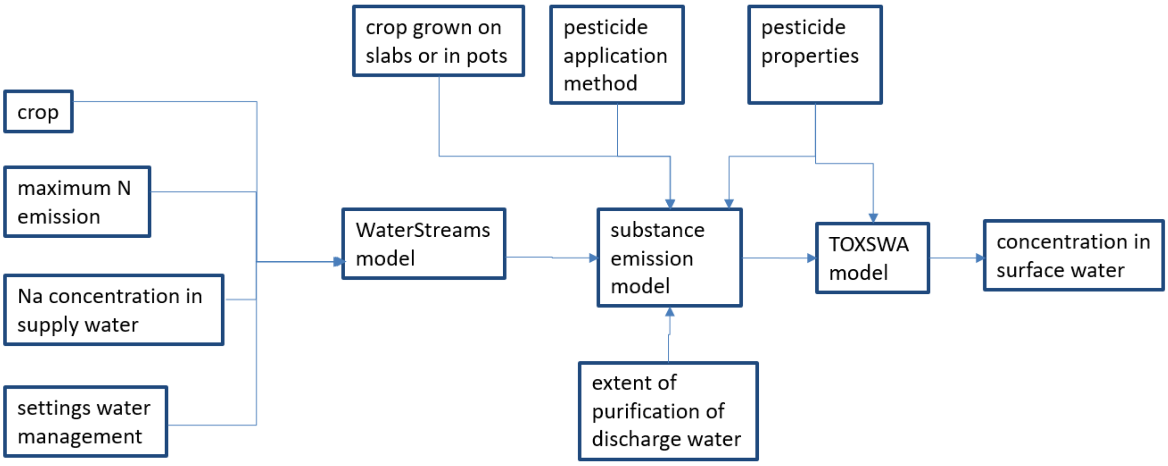


Figure 1 *Schematic presentation of the GEM modelling system for soilless cultivations.*

1.3 Nomenclature of GEM sub-models

Earlier reports described three GEM sub-models, depending on the application method and whether crops were grown on slabs or in pots:

- GEM-A for applications via the nutrient solution (drip irrigation) to crops grown on slabs (stonewool, coir, perlite etc.)
- GEM-B for spray and low-volume mister (LVM) applications to crops grown on such substrates
- GEM-C for spray and LVM applications to crops grown in pots in an ebb/flood system on tables or floors.

The concepts in WSM and in TOXSWA are independent of the type of growth medium and the types of application of the pesticide. However, this is not the case for the concepts in the SEM model; the SEM model allows for six different combinations of crops and application method as shown in Table 1. Considering that only the SEM-model splits into sub-models, in this report we will, instead of using the differentiation between GEM-A, GEM-B and GEM-C, use the acronyms for the SEM model as shown in Table 1.

Table 1 *Combinations of crop systems and application methods in the GEM model and corresponding acronyms of the SEM sub-models. Underlined characters are used in the acronyms.*

Crop grown	Application method	Acronym	
		Old	New
on slabs	drip irrigation	GEM-A	SEM-Sd
	spray	GEM-B	SEM-Ss
	LVM	GEM-B	SEM-Sl
in pots	irrigation water	-	SEM-Pi
	spray	GEM-C	SEM-Ps
	LVM	GEM-C	SEM-Pl

2 WaterStreams Model

2.1 Brief description of WaterStreams Model

Pesticides applied in the greenhouse may be emitted to surface water due to discharge of water to the sewage system or direct discharge to nearby water courses. Although excess irrigation water is mostly reused, it is also partly discharged and applied pesticide may end up in the discharged water. Consequently the volume of discharged water with nutrients and pesticides determines to a large extent the emission to surface water.

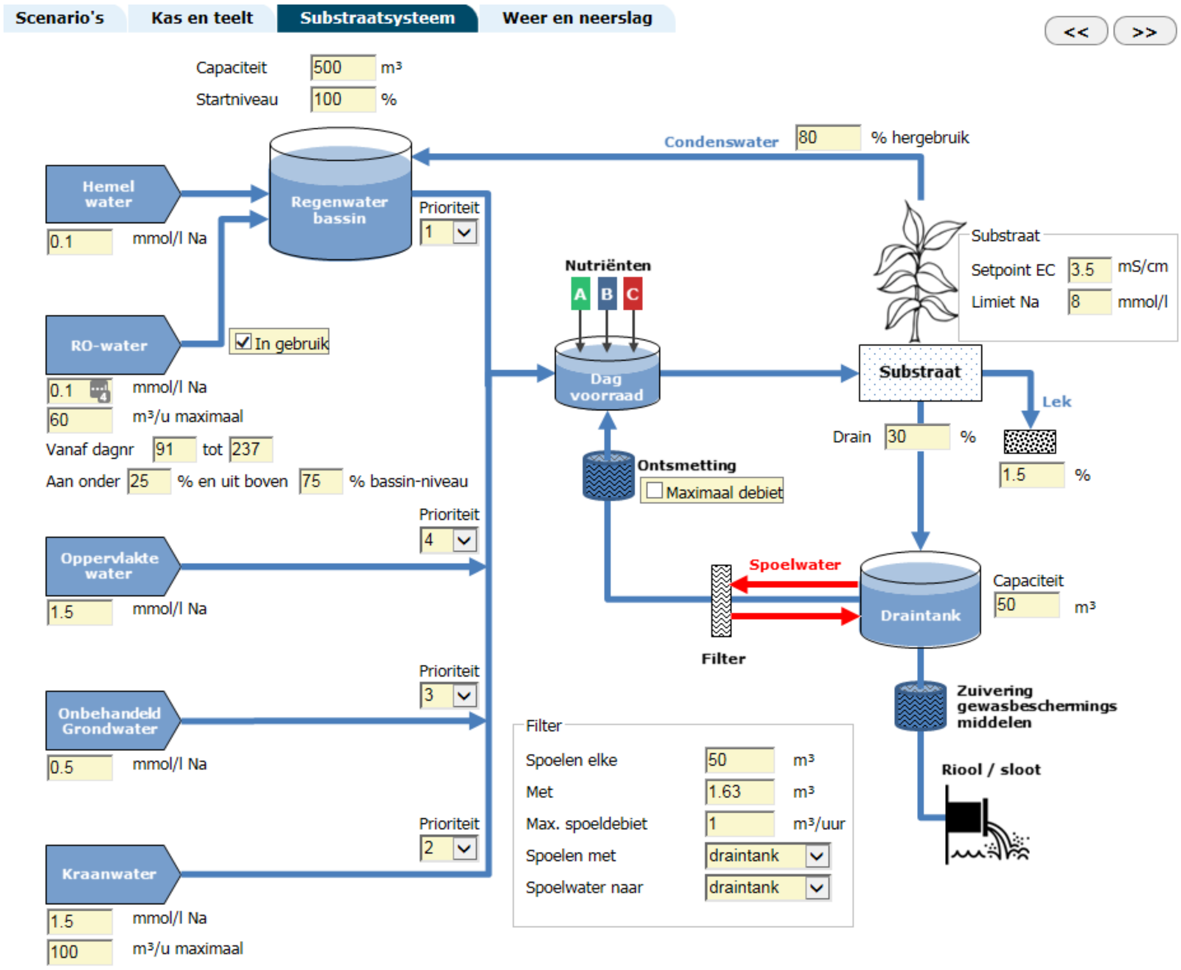
The WaterStreams Model (WSM) was first developed by Voogt et al. (2012) to estimate the total water demand of a soilless grown greenhouse crop. Later on information about emission of nitrogen and water flows were added. The WSM version used in the first editions of GEM is described by Van der Linden et al. (2015). In 2016 a web version of the WSM was released in the Dutch language to provide information on the water demands of individual nurseries to growers and consultants (https://www.wur.nl/nl/nieuws/Telers-kunnen-nu-zelf-hun-waterstromen-berekenen.htm).

In soilless cultures many different crops are grown, and each crop requires a different parameterisation of WSM. Van der Linden et al. (2015) considered it infeasible to parameterise WSM for all possible greenhouse crops that are grown soilless (about 80 in the 2019 DTG list). Therefore they introduced the concept of four emission reference crops: tomato, ficus, rose and sweet pepper. WSM is parameterised for these four reference crops. GEM links a crop selected by the user to the most representative reference crop based on sodium tolerance and water need. From hereon we will refer to the reference crops as *'discharge reference crops'*.

WSM estimates the ingoing and outgoing water fluxes at a standardized commercial nursery. The model uses the crop transpiration model of de Graaf (1988) with some modifications by Voogt et al. (2000) to simulate the water uptake for crop growth. Weather data such as temperature, the sum of radiation, and precipitation, as well as related greenhouse climate data are used as input on an hourly basis. A number of additional parameters are used to calculate the various water fluxes on an hourly basis:

- The volume of the rainwater collection. This is a fundamental parameter, because rainwater is used as the primary water source.
- The chosen years. The timeframe can be selected from a database of measured weather data at Rotterdam Airport. For GEM the years 2000-2006 for consistency reasons (the TOXSWA model is also parameterized for 2000-2006; see also Van der Linden et al., 2015).
- Crop specific parameters. For each of the four discharge reference crops, several crop specific parameter values need to be chosen, e.g. day/night temperature, intensity and duration of artificial lighting, sodium threshold value, and specific sodium uptake.
- Water sources and their sodium concentration.
- Water supply / water uptake ratio, drain fraction, fraction of leakage.
- Filter cleaning water source and system values (Figure 2).

Based on these input data, the WSM calculates hourly usage of rainwater, the daily usage of additional water sources, and the daily produced condensation water. Further, the crop uptake, the required amount of discharge of the nutrient solution and amounts of leakage and filter cleaning water are calculated. Besides water fluxes, also flows and emissions N, P and other elements can be calculated based on the amount of water used. The discharge events are due to sodium accumulation above a crop specific threshold value.



Capaciteit 500 m^3
Startniveau 100 %

Condenswater 80 % hergebruik

Hemel water: 0.1 mmol/l Na

Prioriteit 1

RO-water: ☑ In gebruik
0.1 mmol/l Na
60 m^3/u maximaal
Vanaf dagnr 91 tot 237
Aan onder 25 % en uit boven 75 % bassin-niveau

Prioriteit 4
Oppervlakte water: 1.5 mmol/l Na

Prioriteit 3
Onbehandeld Grondwater: 0.5 mmol/l Na

Prioriteit 2
Kraanwater: 1.5 mmol/l Na
100 m^3/u maximaal

Substraat
Setpoint EC 3.5 mS/cm
Limiet Na 8 mmol/l

Drain 30 %

Lek 1.5 %

Ontsmetting ☐ Maximaal debiet

Draintank: Capaciteit 50 m^3

Filter
Spoelen elke 50 m^3
Met 1.63 m^3
Max. spoeldebiet 1 m^3/uur
Spoelen met draintank
Spoelwater naar draintank

Figure 2 *Screenshot of the input screen for water issues. This figure depicts the main water flows considered in the WaterStreams Model. Five sources of water can be selected (Dutch indication in brackets), i.e. rainwater (hemelwater), osmose water (RO water), surface water (oppervlaktewater), untreated groundwater (onbehandeld grondwater) and tapwater (kraanwater). All of these sources have a different sodium concentration which can be set by the user. The incoming water is collected in the mixing tank (dagvoorraad) and then distributed to the crops. Excess water is collected in the draintank and reused after being filtered and disinfected (Ontsmetting). Deteriorated water and filter water can be discharged to a ditch (sloot) or sewage system (riool) after being treated (to remove pesticide residues).*

Compared to the WSM version described by Voogt et al. (2012), which was also included in the first editions of GEM, the following functionalities were added or adapted:

- Compliance with Nitrogen emission norms was added: until 2027 growers are permitted to discharge a certain amount of nutrient solution up to a certain annual maximum (kg N per ha per year), which may include pesticides;
- Sodium levels of irrigation water can be set by the user;
- Filter rinsing water to be discharged or recirculated and adaptation of the volume of rinsing water is possible;
- Waiting time: an adjustable period between discharge and application of pesticides to lower their emissions was added;
- Adaptations according to the latest insights:
  - Sodium uptake of tomato has been corrected;
  - Electric Conductivity (EC in mS/cm) control on root zone instead of irrigation setpoint, this is in compliance with current grower practices.

The added options will be discussed below. Note that not all implemented changes will be available in GEM4, e.g. the waiting time is not part of GEM4. Also, GEM4 includes a number of predefined scenarios for which the water sources are fixed, hence sodium levels of water sources cannot be set by the user.

2.2 Nitrogen emission norms

In the Dutch greenhouse horticulture most of the crops are grown are grown in soilless systems. Since 1995 (Activiteitenbesluit Milieubeheer, 2012; Besluit Glastuinbouw, 2002), recirculation of the surplus of water given to the plants (drainwater) is mandatory (Van Os, 1998). In the last 10-15 years it appeared that this water surplus is still discharged into surface water or the sewage system including nutrients and pesticides, hampering the improvement of the surface water quality. To comply with the targets set in the EU WFD (Water Framework Directive, 2000), Dutch Governmental bodies and the horticulture employers' organization (LTO Glaskracht) agreed that nitrogen emissions should gradually decrease over time, to near-zero levels in 2027. Measures to reach this zero emission are described in Activiteitenbesluit Milieubeheer of 2012 and 2017. Basically, growers have to stepwise decrease the discharge of nitrogen.

From the emission norms given in Table 2 a translation was made to the allowed annual volume of discharge water (m^3/ha), based on the average concentration nitrate (NO_3) in the supply water and the drain water (Table 3). The resulting maximum discharge flows are given in Table 4.

Table 2 *Nitrogen emission norms (kg.ha-1.year-1) for GEM crops.*

Period	From year	Pepper	Potplant (ficus)	Tomato	Rose, gerbera
2012-2014	2012	200	150	125	250
2015-2017	2015	133	100	83	167
2018-2020	2018	100	75	67	125
2021-2023	2021	67	50	42	83
2024-2027	2024	33	25	21	42
After 2027	2027	0	0	0	0

Activiteitenbesluit Milieubeheer 2012, 2017.

Table 3 *Average nitrate (NO3) concentration in supply and drain per crop group.*

Period	Unit	Pepper	Potplant (ficus)	Tomato	Rose, gerbera
NO_3 in supply	mmol/l	16	14	14	5.5
NO_3 in drain	mmol/l	22	12	30	16
N in drain	kg/m^3	0.31	0.17	0.42	0.22

Note that the volumes in Table 4 have no legal status but are a guideline for growers. If actual nitrate concentrations in drain water are demonstrably lower, a grower can discharge a higher volume of water. While discharge volumes in 2012/2014 could be easily achieved by most of the growers, discharge limits for later periods likely require specific measures.

Table 4 *Maximum discharge of drain water (m3/ha/year) based on N emission norms (Table 2).*

Period	From year	Pepper	Potplant (ficus)	Tomato	Rose, gerbera
2012-2014	2012	650	900	300	1100
2015-2017	2015	450	600	200	750
2018-2020	2018	325	450	150	550
2021-2023	2021	225	300	100	375
2024-2027	2024	112	150	50	187
After 2027	2027	0	0	0	0

In GEM3.3.2 the N emission norms for 2015-2017 or 2018-2020 could be selected. In GEM4, reference periods for 2021-2023 and 2024-2027 have been added. For all periods in Table 4 (except 2012-2014 and after 2027), WSM scenarios have been developed as part of GEM4, simulating water management by a hypothetical grower in order to comply with the relevant discharge limit. This is achieved by varying the filter rinsing setpoints and the sodium concentration threshold in the irrigation water. These parameters are given in Annex 2; other parameters of WSM-V2.0 are listed in Annex 3 and Annex 4 shows the final water discharges of all combinations of discharge reference crops and nitrogen time periods.

2.3 Sodium concentration to be set by the user

The grower’s decision to discharge is mainly due to exceedance of the threshold sodium concentration in the circulating nutrient solution. Threshold values above which discharge is recommended (or was allowed in the past) are available for most of the crops (Besluit Glastuinbouw, 2002). When the concentrations rise above these threshold values, the yield and/or quality of the crop is expected to decrease. In WSM, sources for the irrigation water can be selected (e.g. rainwater or surface water), as well as the sodium concentration of these water sources. The model then calculates the discharge emissions (see Voogt et al., 2012).

For GEM, the water sources and sodium concentrations are set to achieve annual discharge volumes close to the maxima listed in Table 4. While in reality growers may be able to achieve lower discharge volumes, these parameters cannot be changed by the user. GEM calculates exposure concentrations in surface water due to pesticide use in greenhouses which are used in the risk assessment, hence they must be robust and be based on conservative assumptions. Therefore it is assumed that the simulated grower complies with the regulations, but does not achieve lower discharges than required.

2.4 Filter rinsing water

In the last ten years research showed that some growers discharge water used for filter rinsing before the sodium threshold value is reached, mainly because of the fear for loss of quality or quantity of produce. Discharge of filter rinsing water was allowed according to Besluit Glastuinbouw (2002). This regulation was adapted in the Activiteitenbesluit Milieubeheer (2017). The contribution of release of filter rinsing water to nitrogen emission is now included in the maximum emission norms as given in Table 2.

In the past, the rapid sand filter was predominantly used to remove coarse particles, such as algae, roots, leaves, organic matter, sand or substrate particles. This type of filters is automatically rinsed when blocking of the filter occurs and the rinsing water is discharged to surface water or the sewage system. Vermeulen et al. (2010) showed that on average between 100 and 1000 m^3/ha/yr (about 1-10% of the water use) was discharged via the filter rinsing water, being the 2nd largest source of water discharge after discharging to reduce sodium concentration. In some cases, filter rinsing discharge fluxes of more than 2000 m^3/ha/yr occurred. Due to raised awareness of the growers other filter types and other rinsing strategies were developed. New rinsing strategies include:

- The use of automated filters with more frequent rinsing but using much smaller rinsing volumes.
- The use of filters in which particles and water are separated by a 10-40 µm tissue, resulting in a clean water flow with only nutrients, salt and pesticides and a solid waste flow of tissue and particles which can be composted.
- Replacement of drain water as source of rinsing water for basin water (or rainwater). This is possible if sufficient rainwater is available during the entire season.
- Recirculation of the filter rinsing water instead of discharge, by pumping to the dirty water or drain tank where solid particles can precipitate.

In GEM4 there will be options for the user to choose between discharging or to recirculating the filter rinsing water.

In the GEM scenarios, it is assumed that 1.63 m^3 water is used to rinse the filter (approximate value reported by suppliers of sand filters) and rinsing occurs for every 50 m^3 of solution that has passed through the filter (default value). In 0 an overview is given of the filter rinsing setpoints in relation to the sodium concentration in the supply water to achieve the allowed discharge values as given in Table 4.

2.5 Other changes to the WaterStreams Model

During the 4 years of working with WSM and having the model online with more than 300 users, small things in layout or performance were applied between the released version V1.0 (2014) and V2.0 (2018). Below the main additional features as compared to Voogt et al. (2012) are given.

2.5.1 Sodium uptake of tomato

In GEM3.3.2 plant sodium uptake was directly proportional to the transpiration of the crop. In the current version sodium uptake is also proportional to sodium level in the solution in the root environment ($y = 0.172\ x^{0.6548}$ in which y is sodium uptake concentration and x sodium root environment concentration, Voogt & Van Os, 2012). This result in a higher uptake of sodium and less discharge of water.

2.5.2 Calculation of nitrogen discharge

While originally the WSM focus was on sodium and water quality, the current version can also be used to calculate the nitrogen emission (kg N per ha) based on the discharged volumes. This allows growers to assess the impact of various parameters on the volume of discharge. The allowed N (kg/ha) discharged is presented in Table 1 and the related volumes of water in Table 3 (m^3/ha). Calculation is based on average concentrations of nitrate[1].

2.5.3 EC control on root zone instead of irrigation setpoint

The WSM version used in GEM3.3.2 calculates the use of fertilizers based on the EC setpoint of the nutrient solution during irrigation (2.5 – 3.0 mS/cm), hence it is based on the solution going to the plants. In reality, the control of EC takes place on the EC in the root zone (3.0 – 3.5 mS/cm). This is now changed. The impact of this change is that the estimated level of nutrients (a.o. nitrogen) will be slightly higher in the drain water. Consequently less volume per crop per year has to be discharged to obtain the required nitrogen level.

2.5.4 Use of the WaterStreams model outside GEM: web version

The release of the web version in 2016 (http://www.glastuinbouwmodellen.wur.nl/waterstromen/) resulted in many more users, especially growers and consultants who used WSM for calculation of their water flows. It gave them more insight in the water flows with their own specific parameters. WSM was also used in projects to give growers insight in the volume to be discharged and, consequently, in the size of the purification equipment to be bought before January 1, 2018, i.e. the deadline for growers to install purification equipment to purify 95% of the pesticides present in the discharge water before discharging it to surface water or the sewage system (Hoofdlijnenakkoord, 2015).

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[1] Note that nitrate discharge is not based on a transpiration or growth model or a mass balance study. This is not available in literature for nitrogen because of additional biological and chemical processes in the water, substrate and air which affect the total amount of discharged nitrogen.

2.6 Comparison of discharged volumes

The version of WSM-V1.0, 2014 and WSM-V2.0, 2018 were compared using the same parameterisation in both models (Annex 3). An overview of the comparison are given in Table 5. There are four water flows out of the greenhouse water system which may contain pesticides: crop uptake, discharge to reduce sodium level, discharge of filter rinsing water, and condensation water formed at the greenhouse cover. The latter flow is returned to the system as supply water. The following was found for all four crops:

- Water uptake is slightly higher in V2.0 (0.8 – 3.7%), because setpoints temperature were slightly changed (1 °C higher day temperature in the greenhouse);
- Discharge based on sodium is unchanged, because the threshold values are equal;
- Discharge of filter rinsing water increased (9.5 – 20.8%). In V1.0 the discharge strategy in V1.0 was not correct, which resulted in a too low discharge of filter rinsing water;
- In V2.0 discharge timing takes place based on the volume of the draintank at end of the day. In V1.0 this was based on an volume averaged over the day;
- The amount of condensation water decreased slightly (-3.0 – -4.8%), which may be related to the temperature setpoint inside.

Additionally, the effect of the corrected representation of sodium uptake by the tomato crop (section 2.6.1) was tested (Table 5, shaded section), by checking that if the sodium concentration in the supply water increases to 1 mmol/l there is discharge based on sodium. Originally WSM-V1.0 used a Na-uptake of 0.06 mmol/l, now in WSM-V2.0 an uptake of 0.15 mmol/l is used when Na-concentration rises to 1.0 mmol/l according the formula given in chapter 2.6.1. Using the 0.06 mmol/l uptake rate in V1.0 there will be 14.1 l/m^2/yr discharge and in the V2.0 42.6 l/m^2/yr.

Table 5 *Comparison between WSM-V1.0 and WSM-V2.0 on 4 specific water flows and 4 crops.*

Crop	Crop uptake (L/m^2/yr)	Discharge on sodium (L/m^2/yr)	Discharge on filter rinsing water (L/m^2/yr)	Condensation water (L/m^2/yr)
Sweet pepper				
V1.0	666.9	0.0	37.7	82.8
V2.0	687.1	0.0	43.4	79.1
Difference	*3.0%*	*0%*	*15.2%*	*-4.4%*
Potplant (ficus)				
V1.0	463.0	0.0	44.0	92.0
V2.0	480.0	0.0	44.5	89.3
Difference	*3.7%*	*0%*	*1.1%*	*-3.0%*
Rose				
V1.0	832.8	0.0	63.6	181.4
V2.0	839.7	0.0	69.6	175.0
Difference	*0.8%*	*0%*	*9.5%*	*-3.5%*
Tomato (Na = 0.1 mmol/l)				
V1.0	786.6	0.0	19.6	75.0
V2.0	802.4	0.0	23.6	71.4
Difference	*2.0%*	*0%*	*20.8%*	*-4.8%*
Tomato (1mmol/l Na rainwater, original Na-uptake = 0.06 mmol/l)				
V1.0	786.6	14.1	19.6	75.0
V2.0	802.4	42.6	23.6	71.4
Difference	*2.0%*	*201.9%*	*20.8%*	*-4.8%*
Tomato (1mmol/l Na rainwater, adapted Na-uptake = 0.15 mmol/l)				
V1.0	786.6	0.0	20.7	75.0
V2.0	802.4	31.7	24.4	71.4
Difference	*2.0%*	*-- %*	*18.1%*	*-4.8%*

3 Substance emission model for crops grown on slabs

3.1 Introduction

In this chapter pesticide fate processes in the Substance Emission Model for crops grown on slabs (SEM-S) are described. Crops grown in these systems are typically grown in rows. Excess of irrigation water is collected in troughs and this collected water is reused for irrigation. Reuse of irrigation water is obligatory in the Netherlands. Condensation water from the greenhouse roof is collected and reused as irrigation water. Before reuse the water is filtered and disinfected to remove possible pathogens (see Figure 3). Pesticide is applied via the nutrient solution, via spraying or with a low volume mister (Figure 4). In this chapter we describe first the water flows, then the processes controlling pesticide fate in the tanks, followed by the processes in the greenhouse outside the tanks. The processes in the tanks are relevant for all types of pesticide application. Simulated processes include the degradation of the parent substance and the formation of metabolites, sorption, plant uptake and partitioning to roots. The processes outside the tanks are only relevant for spray and LVM applications.

Figure 3 *Young sweet pepper plants on stonewool slabs (left), draintank to collect water from the slabs (middle), storage tanks for rainwater, untreated drain water and disinfected drain water (right).*

Figure 4 *Application via drip irrigation directly into the stonewool slabs (left), normal spraying (middle), LVM (right).*

As described in Section 1.3, the SEM-S model configurations associated with the application types drip irrigation, spraying and LVM will be referred to as SEM-Sd, SEM-Ss, and SEM-Sl, respectively.

In SEM-S pesticide is emitted to surface water by discharge of recirculation water. Discharge of recirculation water is mainly related to exceedance of the Na concentration threshold but also filter cleaning water is discharged. Pesticide enters the recirculation water through:

- Direct application to the irrigation water (SEM-Sd)
- Direct deposition on the slabs or on the troughs used for the drainage flow (SEM-Ss and SEM-Sl)
- Via condensation water flowing from the cover, which is collected in the recirculation water (SEM-Ss and SEM-Sl).

Note further that the discharged water is treated before being released with (an obligatory) minimal removal rate of 95%.

3.2 Configuration of tanks and water fluxes between tanks

The substance emission model conceptualizes the water flow in a greenhouse as a number of interconnected tanks. In general, 'tank' refers to a reservoir in the recirculation water system, simulated explicitly in the model. In most cases the model tanks correspond to actual tanks in the greenhouse. Fate process descriptions for crops grown on slabs (SEM-S) are based on transport via water fluxes between the tanks, as shown in Figure 5. The (recirculated) water is discharged regularly to the surface water. The central part of the system is the 'cultivation tank', i.e. the system of slabs on which the crop is grown with water supply via drip irrigation.

The WaterStreams Model (WSM) calculates the main water fluxes in the greenhouse. The interface between WSM and SEM-S is a file that contains 1-h averages of:

1. the crop evapotranspiration flux,
2. the flux of condensation water to the mixing tank,
3. the water flux from the used-water tank to the wastewater tank,
4. the water flux from the filter to the wastewater tank, and
5. the air temperature in the greenhouse.

Fluxes are provided per ha of cultivation area. The file further specifies the excess of irrigation water, specified as the ratio of the flux to the drain water tank to the flux towards the cultivation tank (set to 0.3 or 0.5, depending on the discharge reference crop type) and the leakage flux out of the cultivation tank (set to 1.5% of the flux towards the cultivation tank). Based on these water fluxes provided by WSM, SEM-S derives all other water fluxes between the differentiated tanks. SEM-S assumes the water volumes in all tanks to be constant except those in the used-water tank and the clean-water tank which may vary between indicated ranges. The corresponding volumes are considered representative for crops grown on slabs. GEM adapts the incoming water flux from the external basin to close the water balance of the system.

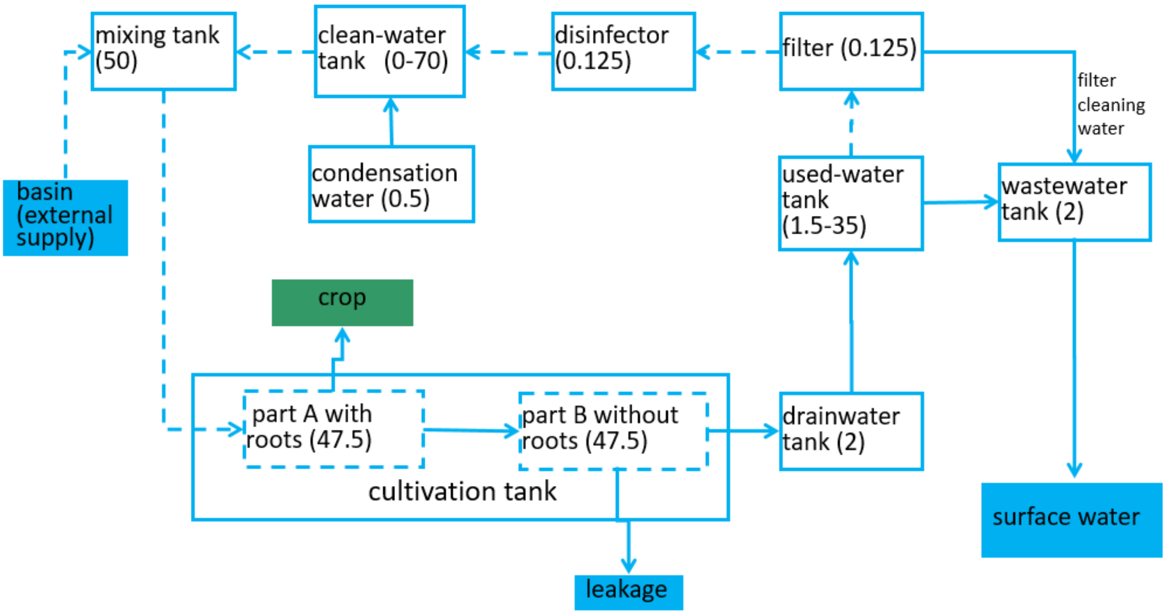

Figure 5 *Layout of the tank systems for SEM-S. The numbers in parentheses are the tank volumes (m^3) scaled to a greenhouse area of 1 ha. Solid arrows are water fluxes provided or prescribed by the WaterStreams model. Dashed arrows are calculated by SEM-S.*

3.3 Processes in the recirculation tanks

The SEM-S model includes both processes in the recirculation water tanks—which are relevant for all application types—and processes in the greenhouse outside these tanks. The latter include processes in the condensation water, which is not considered to be a recirculation tank. This section describes the processes in the recirculation water tanks. In case of pesticide application via the drip irrigation (i.e. for SEM-Sd), only these processes are relevant.

3.3.1 Conservation equations

In each recirculation water tank complete mixing of the substance is assumed. In the earlier SEM versions the cultivation tank was simulated as one tank in which complete mixing was assumed. This tank is now divided into two parts with equal water volumes, referred to parts A and B (Figure 5). This subdivision was motivated by results from a test of SEM-S for pesticide application via the drip irrigation water as described by Wipfler et al. (2020): the observed concentration profile entering the drain water tank could only be described well after sub-dividing the cultivation tank in two tanks of equal volume with root uptake limited to the first tank. The conceptual basis of the subdivision of the cultivation tank is that plant roots tend to concentrate in the areas around the drippers where the nutrient solution enters the slabs (Figure 6). The subdivision leads to more root uptake of the pesticide in the model because the concentration in the part-A tank after an application is higher than in a uniform cultivation tank. Leakage is assumed to take place from part B only (Figure 6).

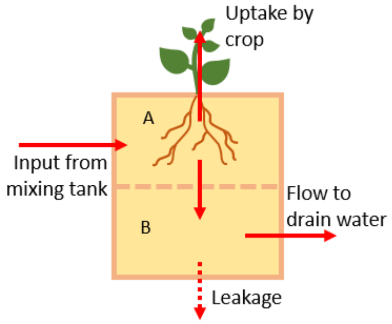

Figure 6 *Conceptual model of subdivision of cultivation tank into parts A and B.*

In addition to recirculation water, the cultivation tank contains substrate (e.g. stonewool), plastic of the surrounding foil and plant roots (only for part-A) to which pesticide can adsorb. Tanks are connected with pipes. Sorption to inner walls of these pipes is considered for the pipes connecting with (parts A and B of) the cultivation tank. These include pipes that provide water to the drippers from the mixing tank (included with part-A of the cultivation tank) and pipes that transport the collected drain water in the troughs to the drain water tank (included with part-B of the cultivation tank).

Possible formation of one or more metabolites by degradation of the parent molecule is considered for all tanks that are part of the recirculation system; metabolites themselves may also be degraded in these tanks. All substances may sorb to the substrate, the plastic of the surrounding foil and the pipes/tubes and both substances may be taken up by the plant roots in the part-A cultivation tank.

The conservation equation for the mass of the parent substance in tank *i* is given by:

$$\frac{dm_{pa,i}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,i}\, c_{w,j} - \sum_{k=1}^{\lambda} Q_{fl,i,k}\, c_{w,i} - V_{w,i}\, k_{t,pa,i}\, c_{w,i} - Q_{up,i}\, TSCF_{pa}\, c_{w,i} + \dot{m}_A \qquad \text{Eqn 1}$$

where $m_{pa,i}$ is the mass of parent substance in tank *i* (kg), ν is the number of incoming water fluxes, $Q_{fl,j,i}$ is the volume rate of water flow ($m^3\ d^{-1}$) from tank *j* to tank *i*, $Q_{fl,i,k}$ is the volume rate of water flow ($m^3\ d^{-1}$) from tank *i* to tank *k* (in which the leakage flow and the flow to the surface water are included although these are formally no flows between system tanks), $c_{w,j}$ is the mass concentration of parent substance in the water of tank j (kg m^{-3}), λ is the number of outgoing water fluxes, $c_{w,i}$ is the mass concentration of parent substance in the water of tank i (kg m^{-3}), $V_{w,i}$ is the volume of water in tank i (m^3), $k_{t,pa,i}$ is the rate coefficient of transformation of the parent substance in tank i (d^{-1}), $Q_{up,i}$ is the volume rate of uptake of water by plant roots (m^3 d^{-1}) which is zero for all tanks except the part-A cultivation tank, and $TSCF_{pa}$ is the transpiration stream concentration factor (-) of the parent. We refer to Briggs et al. (1982) for further detail on the TSCF factor. The WSM model provides the volume rates assuming a surface area of 1 ha so also the tank volumes refer to 1 ha.

$\dot{m}_A$ (kg d^{-1}) is the applied mass rate of the parent compound. After application mass is added to the recirculation water. It depends on the type of application to which tank the mass is added. The model assumes that the application of a pesticide is not instantaneous: it is assumed that an application takes 2 h. During each time step within the application time period, an equivalent amount of pesticide is introduced. For application via drip irrigation this mass is added the mixing tank. For spray and LVM applications some additional processes outside the recirculation water tanks have to be accounted for as explained in Section 3.4.

The conservation equation for the mass of the metabolite in each tank with number i is similar to that of the parent but includes also the formation of the metabolite from the parent and has not application related term. It is given by:

$$\frac{dm_{me,i}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,i}\, C_{w,j} - \sum_{k=1}^{\lambda} Q_{fl,i,k}\, C_{w,i} - V_{w,i}\, k_{t,me,i}\, C_{w,i} + V_{w,i}\, \chi\, \frac{m_{mol,me}}{m_{mol,pa}}\, k_{t,pa,i}\, c_{w,i} - Q_{up,i}\, TSCF_{me}\, C_{w,i} \qquad \text{Eqn 2}$$

where $m_{me,i}$ is the mass of parent substance in tank i (kg), $C_{w,j}$ is the mass concentration of metabolite in the water of tank j (kg m^{-3}), $C_{w,i}$ is the mass concentration of metabolite in the water of tank i (kg m^{-3}), $k_{t,me,i}$ is the rate coefficient of transformation of the metabolite (d^{-1}) in tank i, χ is the molar fraction (-) of parent that is transformed into the metabolite, $m_{mol,me}$ is the molar mass of the metabolite (kg mol^{-1}), $m_{mol,pa}$ is the molar mass of the parent (kg mol^{-1}), and $TSCF_{me}$ is the $TSCF$ (-) of the metabolite. Please note that upper case C is used for the metabolite and lower case c for the parent.

The rate coefficients $k_{t,pa,i}$ and $k_{t,me,i}$ are temperature dependent. This dependency is described by the Arrhenius equation. The molar enthalpy for this process is to be provided by the user, with a default value of 64 kJ mol^{-1}. It is assumed that these rate coefficients measured at an arbitrary reference temperature (usually 20°C) are equal for all tanks except the disinfector tank for which other values of rate coefficients can be provided. The temperature of the cultivation and drainage tanks is assumed to be equal to the air temperature in the greenhouse. The temperature of the other tanks is assumed to be 2°C colder because these other tanks are located in a separate part of the greenhouse.

For the disinfector tank, the half-life approach to calculate transformation is not in line with how the removal of pesticide by an disinfection unit is generally measured. Also, this approach may lead to numerical errors due to the short residence time in this tank. Therefore, an option was introduced to calculate transformation in the disinfector tank based on a removal fraction: the fraction of substance that is removed in the tank as relative to the incoming mass. This form of pesticide removal is not influenced by temperature.

3.3.2 Adsorption in the cultivation tank

For all tanks, except the cultivation tanks, the concentrations of substance in water are calculated as the quotient of the mass in the tank and the volume of water in the tank.

In the part-A cultivation tank, the concentration is reduced by the following partitioning processes:

- Partitioning into the roots
- Sorption to the substrate material (stonewool, coir etc.)
- Sorption to the surrounding plastic foil
- Sorption to the different types of plastic tubes between the mixing tank and the part-A cultivation tank.

In the part-B cultivation tank no partitioning into the roots is considered and sorption to the tubes is limited to one type of tubes (PVC tubes).

This leads to the following relationship for the mass of parent substance present in the part of the system that starts where the water leaves the mixing tank and that ends where the water leaves the part-A cultivation tank:

$$m_{pa,culA} = V_{w,culA}\, c_{w,culA} + M_{sub,culA} K_{sub}\, c_{w,culA} + f_{foil} M_{foil,culA} K_{foil}\, c_{w,culA} + M_{roots}\, RCF\, c_{w,culA} + \left(\sum_{i=1}^{3} L_i\, S_i + \sum_{i=1}^{3} L_i\, p_i\, K_{tube,i}\right) c_{w,culA} \qquad \text{Eqn 3}$$

where $m_{pa,culA}$ is the mass of parent substance in the part-A cultivation tank (kg), $V_{w,culA}$ is the volume of water in this tank (m^3), $c_{w,culA}$ is the mass concentration of parent substance in this tank (kg m^{-3}), $M_{sub,culA}$ is the dry mass of substrate in this tank (kg), K_{sub} (m^3 kg^{-1}) and K_{foil} (m^3 kg^{-1}) are the sorption coefficients of the substrate and the foil, respectively, f_{foil} is a factor (-) to account for incomplete contact between foil and the water in the tank (set at 0.5), *RCF* is the root concentration factor (m^3 kg^{-1}), $M_{foil,culA}$ is the mass of foil in this tank (kg), M_{roots} is the mass of wet roots in this tank (kg), and with

$$\sum_{i=1}^{3} L_i\, S_i = L_{PVC}\, S_{PVC} + L_{pei}\, S_{pei} + L_{pec}\, S_{pec} \qquad \text{Eqn 4}$$

$$\sum_{i=1}^{3} L_i\, p_i\, K_{tube,i} = L_{PVC}\, p_{PVC}\, K_{tube,PVC} + L_{pei}\, p_{pei}\, K_{tube,pei} + L_{pec}\, p_{pec}\, K_{tube,pec} \qquad \text{Eqn 5}$$

where *L* is the length of a class of pipes/tubes (m), *S* is the inner surface area (m^2) of a class of pipes/tubes, *p* is the mass per length (kg/m) of a class of pipes/tubes, K_{tube} is the sorption coefficient (m^3/kg) of a class of pipes/tubes and where the subscripts *PVC*, *pei* and *pec* indicate the PVC transport pipes, polyethene irrigation tubes and polyethene capillary tubes, respectively[2]. The PVC transport pipes are the main conducts (both for transport of water to the cultivation tank and for transport of water from the cultivation tank to the drainage tank). The polyethene irrigation and capillary tubes are used for distributing the irrigation water to the drippers that provide each plant with irrigation water.

Measurements of K_{foil} by batch incubation will give the sorption to the two sides of the foil whereas the pesticide or its metabolite in the slab system can sorb only to the inner side. Therefore K_{foil} is multiplied with 0.5 in the model.

The root concentration factor *RCF* is based on Briggs et al. (1982) who established the following relationship between partitioning of pesticides into roots and the octanol-water partition coefficient:

$$RCF = 8.2 \times 10^{-4} + 3.02 \times 10^{-5}\ (K_{ow})^{0.77} \qquad \text{Eqn 6}$$

where the *RCF* (m^3/kg) is defined as the concentration in the roots divided by the concentration in the water (with concentration in roots defined as mass of pesticide in roots per mass of wet roots), and K_{ow} is the octanol-water distribution coefficient (-).

The equations for the mass of metabolite in part A of the cultivation tank are identical to the above three equations.

The equations for the mass of pesticide and its metabolite in the part-B cultivation tank are similar to Eqn 3 with the exception that the terms for sorption to the polyethene tubes and on the root partitioning are not included. Hence, for the part-B cultivation tank, the following equation for the parent applies:

$$m_{pa,culB} = V_{w,culB}\, c_{w,culB} + M_{sub,culB} K_{sub}\, c_{w,culB} + f_{foil} M_{foil,culB} K_{foil}\, c_{w,culB} + \left(L_{PVC} S_{PVC} + L_{PVC} p_{PVC} K_{tube,PVC}\right) c_{w,culB} \qquad \text{Eqn 7}$$

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[2] Note that $K_{tube,pei}$ and $K_{tube,pec}$ have the same value.

where the subscript 'culB' refers to the part-B cultivation tank. Again, the equation for the metabolite is identical to that for the parent. It is assumed that the mass of dry substrate, the mass of foil and the length of the PVC tubes are equally divided over parts A and B.

The numerical solution of the rate equations (Eqns 1 and 2) is done with explicit Euler's method, which assumes that the rates are constant during the integration interval. The time step is fixed to 1 min.

A complete list of parameter values for the parameters in the equations above can be found in Annex 7.

3.3.3 Purification of discharged water

The discharged water must be purified before emission to the surface water according to the Dutch regulations (Activiteitenbesluit Milieubeheer 2017). This is simulated in the model by multiplying the concentrations that enter the surface water by a purification reduction factor. Hence, the mass flux of pesticide (or its metabolite) to the surface water, J_{sw} (kg d^{-1}), is described by:

$$J_{sw} = \varphi \ Q_{fl,ww} \ c_{w,ww} \qquad \text{Eqn 8}$$

where φ is the purification reduction factor (-), $Q_{fl,ww}$ is the volume rate of water flow (m^3 d^{-1}) from the wastewater tank to the surface water, $c_{w,ww}$ is the mass concentration of pesticide or metabolite (kg m^3) in the wastewater tank.

3.4 Processes in the greenhouse outside the recirculation tanks

3.4.1 Main concepts

After application by spraying or LVM (i.e. in SEM-Ss and SEM-Sl), pesticide can enter the water in the recirculation tanks via three routes:

- Direct contamination of the water in the cultivation tank due to e.g. spray liquid dripping from the plant or flowing from the stem into the 10 × 10 cm substrate blocks in which the plants were introduced into the system[3]
- Direct contamination by deposition of spray or LVM droplets onto the troughs that transport the drainage water of the cultivation tank to the drain water tank
- Via the condensation water on the roofs that flows into the clean-water tank (the condensation water on the walls of the greenhouse is not included because this flows into the soil and thus does not become part of the recirculating water).

Implementing the first two routes in the model is straightforward: the corresponding mass of pesticide is simply added to the cultivation tank and to the drain water tank. The model assumes that the pesticide dissolves instantaneously. The condensation-water route is more complex as is illustrated by the scheme of Figure 7. After a pesticide application, part of the dose is deposited on the plants, the floor and the roof. These deposits volatilise and thus contaminate the air in the greenhouse. The deposit on the roof may also dissolve directly into the condensation water stream. The deposits on the plant and the floor may also dissipate due to other processes than volatilisation (not shown in the scheme). Wash-off from the plants is not considered. The model includes exchange fluxes between the air in the greenhouse and the condensation water due to partitioning. Furthermore, pesticide is transported from the greenhouse into the outside air by ventilation.

As indicated by Figure 7, there are no fluxes from any of the recirculation water tanks to the greenhouse air. Since metabolite formation is only considered in the recirculation water, metabolites

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[3] It is common practice to grow young plants in blocks of 10 by 10 cm and later on place these blocks on the larger slabs. In Figure 3 these blocks are shown in the photo to the left.

do not occur outside the tanks. Therefore, the remainder of this chapter deals with the parent substance only.

In line with the scheme depicted in Figure 7, the model includes simulation of the following quantities as a function of time:

- The mass of pesticide on the plants per surface area of greenhouse, A_p (kg m^{-2})
- The mass of pesticide on the floor per surface area of greenhouse, A_f (kg m^{-2})
- The mass of pesticide in the greenhouse air per surface area of greenhouse, A_a (kg m^{-2})
- The mass of pesticide on the roof per surface area of greenhouse, A_r (kg m^{-2})
- The mass of pesticide in the condensation water on the greenhouse roof per surface area of greenhouse, $A_{w,cds}$ (kg m^{-2})
- The concentration in the greenhouse air, $c_{a,g}$ (kg m^{-3})
- The concentration in the condensation water on the roof, $c_{w,cds}$ (kg m^{-3})

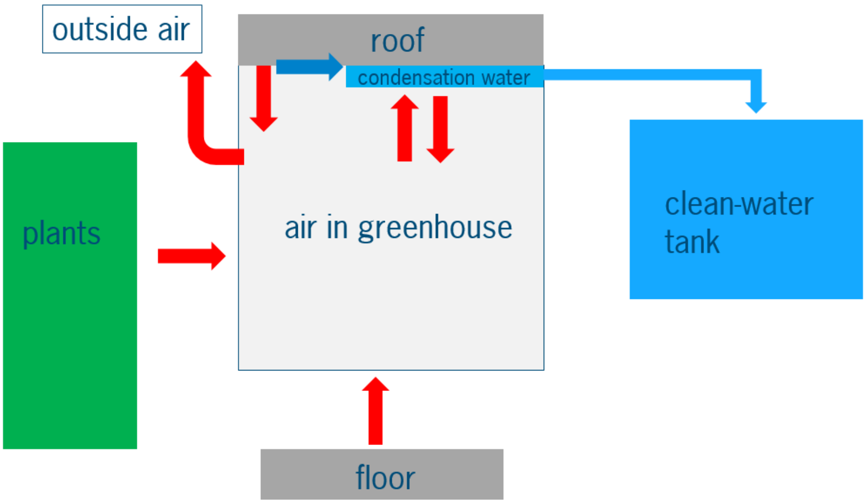

Figure 7 *Schematic representation of the processes related to the concentration of the parent substance in the air of the greenhouse in for spray and LVM applications (SEM-Ss and SEM-Sl). The condensation water is assumed to be present on the roof and is regularly discharged into the clean water tank. The red arrows are gas fluxes of the substance and the blue arrows are water fluxes that carry substance.*

3.4.2 Distribution of the dose after spray or LVM applications

The model assumes that the spray or LVM application of a pesticide is not instantaneous but occurs over a period of 2 h. During each time step within the application period, an equivalent amount of pesticide is introduced and distributed over the different pools as described below.

During application, the substance is distributed over several locations in the greenhouse. The exact distribution fractions are dependent on the application type and crop. Since it is infeasible to provide estimates of this distribution for all possible crops, Van der Linden et al. (2015) introduced the concept of the deposition reference crops: representative crops which represent the variation of application distribution fractions for real crop. They used five reference crops: (1) cut flowers & pot plants, (2) lettuce & radish, (3) tomato & cucumber, (4) rose & gerbera and (5) very young plants. For each of these categories they estimated the fractions of the dose deposited on the plants and the floor. For GEM4, it was decided to not differentiate between crops since data on crop deposition in greenhouses is very rare and associated uncertainty is high. Also, the deposition fractions were reconsidered, in part because deposition on additional surfaces was introduced (e.g. the roof). The deposition fractions represent a realistic worst-case scenario that results in a relatively high discharge concentrations (see als0 Annex 5).

Spray applications

It is assumed that a spray application does not lead to immediate contamination of the air or the condensation water. Hence, unless pesticide residues are left from previous applications, the air and condensation water are free of substance immediately after the start of a spray application.

The initial distribution between crop, floor, roof, troughs and mats (slabs) is given in Table 6. These numbers are based on a 40/60 division for the depositions on the crops and the floor (see Annex 5) plus the deposition percentages of the last three items as proposed by Boesten et al. (2019). As indicated, the dose is applied over 2 hrs.

Table 6 *Initial distribution of pesticide after spray applications.*

Fraction of applied dose for spray drift applications	
Deposited on crop surface	0.3944
Deposited on floor	0.5916
Deposited on roof	0.0010
Dripped into slabs	0.0100
Deposited on troughs	0.0030

Note that in the event of a spray application $\dot{m}_A$ in Eqn 1 is:

$$\dot{m}_A = Ai * Sgh * (f_{sl} + f_{tr}) \qquad \text{Eqn 9}$$

for the cultivation tank, part A. Where Ai is the applied areic mass rate (kg m^{-2} d^{-1}), *Sgh* is the surface area of the greenhouse (10^4 m^2), f_{sl} is the deposited fraction on the slabs and f_{tr} is the deposited fraction on the throughs.

LVM applications

Immediately after the start of an LVM application the concentration in the air is considered to be equal to the concentration of a saturated vapour, $c_{a,sat}$ (kg m^{-3}), which is calculated from

$$c_{a,sat} = \frac{m_{mol}\, P_{sat}}{R\, T} \qquad \text{Eqn 10}$$

where m_{mol} is the molar mass (kg mol^{-1}), P_{sat} is the saturated vapour pressure (Pa), *R* is the gas constant (8.31 J mol^{-1} K^{-1}) and *T* is the absolute temperature (K) in the air of the greenhouse. The application of pesticide does not include direct deposition on the condensation water. So immediately at the start of the first LVM application the condensation water is free of pesticide.

The saturated vapour pressure is a function of temperature:

$$P_{sat} = P_{sat,ref}\ exp\left(\frac{-E_v}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \qquad \text{Eqn 11}$$

where T_{ref} is a reference temperature (K) set at 293.15 K, $P_{sat,ref}$ is the P_{sat} at the reference temperature and E_v is the molar enthalpy of vaporisation (kJ mol^{-1}) with a default value of 96 kJ mol^{-1}.

The remaining part of the dosage after an LVM application is distributed between crop, floor, roof, troughs and slabs as shown in Table 7 (see Annex 4 for justification). Note that the applied mass is considered to be applied in a timeframe of 2 hr.

Table 7 *Initial distribution of pesticide after LVM applications. Fractions apply to the applied mass per surface area of greenhouse (A_i) minus the mass per surface area of greenhouse corresponding with the saturated vapour concentration ($A_{a,sat}$).*

Fraction of (A_i- $A_{a,sat}$) for LVM applications	
Deposited on crop surface	0.3908
Deposited on floor	0.5862
Deposited on roof	0.0100
Dripped into slabs	0.0100
Deposited on troughs	0.0030

Note that in the event of a LVM application $\dot{m}_A$ is then calculated using Eqn 9.

3.4.3 The pesticide fluxes in the gas phase

The volatilisation rate from the plant surface in SEM-S is calculated as

$$J_{v,p} = b \ \ LAI \ \frac{A_p}{A_{p,i}} \ \ \frac{F c_{a,sat} - c_{a,g}}{r_{a,p}} \qquad \text{Eqn 12}$$

where $J_{v,p}$ is the (areic) mass flux of pesticide (kg m^{-2} d^{-1}) from the plants to the air, *b* is a factor (-), *LAI* (-) is the leaf area index[4] of the selected crop, $A_{p,i}$ is the mass of pesticide on the plants per surface area of greenhouse (kg m^{-2}) immediately after application (*i* for initial)[5], *F* is a factor (-) describing the deviation of the concentration in the gas phase at the plant surface from $c_{a,sat}$ (*F* is set to 0.2), $c_{a,g}$ is the mass concentration in the greenhouse air (kg m^{-3}), and $r_{a,p}$ is the laminar boundary layer resistance (d m^{-1}) at the plant surface. The factor *b* is set to 2 for spray applications (SEM-Ss) and 1 for LVM applications (SEM-Sl) because spray applications deposit pesticide both on top and at the underside of the leaves whereas LVM applications only lead to presence on top of the leaves. This equation applies with the restriction that only positive values of the flux occur (so no deposition), so if $c_{a,g} < F\, c_{a,sat}$ then the flux is set to zero[6].

The volatilisation rate from the floor is calculated as:

$$J_{v,f} = f_{con} \frac{A_f}{A_{f,i}} \frac{c_{a,sat} - c_{a,g}}{r_{a,f}} \qquad \text{Eqn 13}$$

where $J_{v,f}$ is the mass flux of pesticide (kg m^{-2} d^{-1}) from the floor to the air, f_{con} is the fraction (-) of the floor surface that is contaminated with spray or LVM deposits, estimated at 0.5, $A_{f,i}$ is the mass of pesticide on the floor per surface area of greenhouse (kg m^{-2}) immediately after application[5], and $r_{a,f}$ is the laminar boundary layer resistance (d m^{-1}) at the floor surface.

The mass flux for exchange between the condensation water and the greenhouse air, $J_{a/w}$ (kg m^{-2} d^{-1}), is described by

$$J_{a/w} = GAI \frac{(K_H c_{w,cds} - c_{a,g})}{r_{a,w,cds}} \qquad \text{Eqn 14}$$

where *GAI* is the Glass Area Index (-) defined as the surface area of roof divided by the surface area of the greenhouse, K_H is the Henry coefficient (-), $c_{w,cds}$ is the mass concentration in the condensation water (kg m^{-3}) and $r_{a,w,cds}$ is the laminar boundary layer resistance (d m^{-1}) at the condensation water surface. This formulation has the consequence that the value of $J_{a/w}$ is positive if the flux is from the condensation water to the air (consistent with the positive signs of $J_{v,p}$ and $J_{v,f}$). The Henry coefficient

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[4] The LAI in greenhouses is defined as the sum of the one-sided surface areas of the leaves divided by the surface area of the greenhouse.

[5] In the implementation the applied mass is applied over a timeframe of 2 hrs. So, instead of having one initial applied mass the accumulated mass after 2 hrs is recorded. This accumulated mass on the crop surface/floor is slightly lower than the total applied mass because of the dissipation processes that occurred in these 2 hrs.

[6] Note that occasionally the saturated vapor pressure may be exceeded due to decrease in temperature of the greenhouse air. If this occurs surplus substance is assumed to be deposited on the plant leaves.

K_H is the ratio of the concentration in the gas phase divided by the concentration in the liquid phase and is estimated from the ratio of the saturated concentrations of both phases (based on the saturated vapour pressure and water solubility). This K_H depends on temperature because both the saturated vapour pressure and the water solubility depend on temperature. The temperature-dependence of the water solubility is described by:

$$c_{w,sol} = c_{w,sol,ref}\ exp\left(\frac{-E_d}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \qquad \text{Eqn 15}$$

where $c_{w,sol}$ is the water solubility (kg m^{-3}), $c_{w,sol,ref}$ is the $c_{w,sol}$ at the reference temperature and E_d is the molar enthalpy of dissolution (kJ mol^{-1}) set at 27 kJ mol^{-1}.

The mass flux of pesticide volatilisation rate from deposit on roof, $J_{v,r}$ (kg m^{-2} d^{-1}), is described by

$$J_{v,r} = g\ GAI\ \frac{A_r}{A_{r,i}}\left(\frac{c_{a,sat} - c_{a,g}}{r_{a,r}}\right) \qquad \text{Eqn 16}$$

where g is a proportionality factor (-) to account for the fact that probably only a very small fraction of the roof is covered by this deposit, $A_{r,i}$ is the initial value of A_r immediately after application[7] and $r_{a,r}$ is the laminar boundary layer resistance (d m^{-1}) at the roof surface. The factor g is set at 0.01 (Boesten et al., 2019).

Based on measurements by Stanghellini (1987) on heat exchange between plant leaves and greenhouse air, we decided to use r_a = 200 s/m = 2.32 $\times 10^{-3}$ d/m for all exchange processes between surfaces (leaves, floor, roof, pots) and the air.

The ventilation flux, J_{vent} (kg m^{-2} d^{-1}) is calculated as

$$J_{vent} = H_a\ N_{vent}\ c_{a,g} \qquad \text{Eqn 17}$$

in which H_a is the volume of air per surface area of greenhouse (i.e. 6 m) and N_{vent} is the ventilation rate coefficient (d^{-1}) which is set at 50 d^{-1} (based on van der Linden et al., 2015).

3.4.4 The pesticide fluxes to and from the condensation water

The mass flux for the dissolution of pesticide deposited onto the roof, $J_{dis,r}$ (kg m^{-2} d^{-1}), is described by

$$J_{dis,r} = \alpha\, q_{cds} \frac{A_r}{A_{r,i}}\left(c_{w,sol} - c_{w,cds}\right) \qquad \text{Eqn 18}$$

where α is a proportionality factor (-), q_{cds} is the volume flux of condensation water (i.e. volume rate per surface area of greenhouse, m d^{-1}) flowing to the mixing tank, A_r is the mass per surface area deposited onto the roof surface (kg m^{-2}), and $A_{r,i}$ is the initial value of A_r. Hence, $J_{dis,r}$ is described as a convective flux which is directly proportional to q_{cds}. The procedure to describe the ratio of $A_r / A_{r,i}$ for multiple applications is the same as described at the end of the previous section. The default value of α is 0.07 (Boesten et al., 2019).

The mass flux of pesticide from the pool of condensation water to the clean-water tank (J_{cds}, kg m^{-2} d^{-1}) is described by:

$$J_{cds} = q_{cds}\ c_{w,cds} \qquad \text{Eqn 19}$$

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[7] See remark above on the implementation of the initial deposition for the crop surface and the roof.

3.4.5 The rate equations for amounts on plants, floor, roof and in air and condensation water in SEM-S

The rate equation for the areic mass on the plant surface A_p is given by

$$\frac{dA_p}{dt} = -J_{v,p} - k_p\ A_p + J_{A,P} \qquad \text{Eqn 20}$$

where k_p is the coefficient for degradation on the plant canopy (d^{-1}) with a default value corresponding with a half-life of 10 d. The coefficient k_p does not depend on temperature. $J_{A,P}$ is the areic mass rate applied to the crop surface (kg m^{-2} d^{-1}). $J_{A,P}$ is zero except during a pesticide application, when it is equal to the applied dose times the deposited fraction on the crop surface applied in 2 hrs.

The rate equation for the areic mass on the floor A_f is given by

$$\frac{dA_f}{dt} = -J_{v,f} - k_f\ A_f + J_{A,F} \qquad \text{Eqn 21}$$

where k_f is the coefficient for degradation on the floor (d^{-1}) with a default value corresponding with a half-life of 100 d. The coefficient k_f does not depend on temperature. $J_{A,F}$ is the areic mass rate applied to the floor (kg m^{-2} d^{-1}), $J_{A,F}$ is zero except in case of an pesticide application, then it is equal to the applied dose times the deposited fraction on the floor applied in 2 hrs.

The rate equation for the areic mass on the roof A_r is given by:

$$\frac{dA_r}{dt} = -J_{dis} - J_{v,r} + J_{A,R} \qquad \text{Eqn 22}$$

where $J_{A,R}$ is the areic mass rate applied to the roof (kg m^{-2} d^{-1}). $J_{A,R}$ is zero except in case of an pesticide application, when it is equal to the applied dose times the deposited fraction on the roof applied in 2 hrs.

The rate equation for the areic mass in the greenhouse air A_a is given by:

$$\frac{dA_a}{dt} = +J_{a/w} + J_{v,p} + J_{v,f} + J_{v,r} - J_{vent} + J_{A,A} \qquad \text{Eqn 23}$$

So it is assumed that degradation in the air does not play a role. Note further that in case of LVM application, the applied mass is assumed to volatilize in the greenhouse air instantaneously and that, when saturated vapour pressure is reached, deposition of the parent substance occurs according to the fractions listed in Table 7[8]. The associated flux is indicated by $J_{A,A}$ in Eqn 23.

The rate equation for the areic mass in the condensation water $A_{w,cds}$ is given by:

$$\frac{dA_{w,cds}}{dt} = -J_{a/w} + J_{dis} - J_{cds} - H_{w,cds}\ k_{w,cds}\ c_{w,cds} \qquad \text{Eqn 24}$$

where $H_{w,cds}$ is the volume of condensation water per surface area of greenhouse (i.e. 0.0532 mm) and $k_{w,cds}$ is the degradation rate coefficient of the substance in the condensation water (d^{-1}). This coefficient depends on temperature using the Arrhenius equation; it is assumed that the temperature of the condensation water equals the air temperature in the greenhouse.

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[8] Also, due to temperature fluctuations the saturated vapor pressure may be exceeded, which will occasionally lead to deposition on the crop surface.

The concentrations in the greenhouse air and in the condensation water are calculated from A_a and A_w using:

$$A_a = H_a c_{a,g} \qquad \text{Eqn 25}$$

$$A_{w,cds} = H_{w,cds} c_{w,cds} \qquad \text{Eqn 26}$$

Where H_a is the volume of air per surface area of greenhouse (m^3 m^{-2}). The numerical solution of the rate equations consisted of explicit Euler's method so assuming that the rates are constant during the integration interval. The time step was fixed to 1 min.

The explicit scheme for numerical solution may in rare situations lead to negative values of the quantity that is integrated. This was prevented using an iteration procedure that reduced the rate of change such that the integrated quantity does not become negative (see Annex 6).

3.5 Expected effects of changes in SEM-S implemented for GEM4

From a regulatory point of view, it is interesting to assess the likely impact of the changes in SEM-S on the emission concentrations. The main changes are:

1. Sorption to the slab material (e.g. stonewool), surrounding foil, and the walls of the irrigation pipes have been added, as well as partitioning into the roots (leading to decreased emission concentrations),
2. The amounts of pesticide in the air and condensation water immediately after a spray or LVM application have been strongly reduced (from 8% to 0% for spray and from 35% to about <1% for LVM applications, leading to decreased emission concentrations),
3. The concentration in the air at the plant surface has been reduced from 100% to 20% of the saturated vapour concentration (leading to decreased emission concentrations),
4. In case of spray or LVM applications, small parts of the dose (0.1-1%) are deposited during application on (a) the slabs, (b) the troughs that collect the drainage water of the slabs, and (c) the roof (leading to increased emission concentrations; for spray and LVM applications of non-volatile pesticides, these direct depositions are the only sources of water contamination)
5. After spray or LVM applications, about 40% of the dose is deposited onto the plants and about 60% on the floor, compared to 55-80% on the plants and 10-20% on the floor in the previous version (leading to increased emission concentrations)
6. The cultivation tank is subdivided into two parts with equal volume, with uptake of water and pesticide by the roots of the crop is restricted to the first part (leading to decreased emission concentrations).

For applications via the irrigation water there are only changes that lead to decreases in emission concentrations. For spray and LVM applications the changes may both lead to decreases and increases and it is a priori difficult to predict the overall direction of the changes.

4 Substance emission model for crops grown in pots

4.1 Introduction

In this section processes related to crops grown in pots in an ebb/flood system, i.e. grown on tables or floors are described (Figure 8). Similar to crops grown in slabs, for these type of cropping systems excess of irrigation water is collected in troughs and this collected water is reused for irrigation. Crops grown in pots are irrigated every two or three days in a approximately 0.5 hr event: a water layer of about 5 cm is formed on the tables which gradually drains away over a period of 15-20 min. Also, condensation water from the greenhouse roof is collected and added to be reused as irrigation water. Before reuse the water is filtered and disinfected to remove possible pathogens. Pesticide is applied via the nutrient solution (applied with a flooding system), via spraying or with a low volume mister.

Crops in pots are generally grown in peat or other types of substrate material. For convenience, we will refer to all this material as ‘soil’ because of the presumably similar characteristics of the substrate material in the pots.

Pesticides applied on crops grown in pots on floors will be assessed according to the SEM-P concepts. Crop grown in pots on tables will follow the SEM-P concepts as described in this chapter.

Similar to SEM-S, in SEM-P pesticides can be applied by three methods: with the irrigation water (SEM-Pi), by spraying (SEM-Ps), by LVM application (SEM-Pl). Pesticide can enter the recirculation tanks by the following routes:
- by application to the irrigation water (SEM-Pi)
- deposition onto the tables during application (SEM-Ps and SEM-Pl)
- via condensation water flowing from the roof (SEM-Ps and SEM-Pl).

The sections below describe the concepts and equations used in SEM-P. A complete list of parameter values can be found in Annex 7 including a list of crop specific parameters.

Figure 8 *Pot plants on tables (left and middle), and on concrete floors (right).*

4.2 Configuration of tanks and water fluxes between tanks

Since insufficient information is available on representative volumes of the tanks for ebb/flood systems, we assume that the volumes are the same as for SEM-S (as shown in Figure 5). In SEM-P the equivalent of the cultivation tank is the irrigation water on the tables. In the model, water flow through this tank is continuous at a rate equal to the crop evapotranspiration (as in SEM-S). However the actual irrigation procedure is different.

The interface between the WSM and SEM-P is identical to that of SEM-S (see Section 3.1). However, for crops grown in pots, the uptake of water from the cultivation tank takes place by flow of water into the pots (due to capillary rise in the pots) during the 0.5 h irrigation period (so not continuously by the roots as in SEM-S). In the model however, plant uptake takes places continuously and the volume of water in the cultivation unit is constant.

A further difference between SEM-P and SEM-S with respect to the water flow is that there is no subdivision of the cultivation tank in SEM-P because there is no reason to subdivide the ebb-flood irrigation water in SEM-P.

Rationale for using the same WSM water flows and conditions as for slabs (SEM-S)
A water layer of 5 cm corresponds with 500 m^3 ha^{-1} whereas the volume of the cultivation tank is assumed to be 95 m^3 ha^{-1} (Figure 5). This seems at first glance inconsistent. However, it is possible that the irrigation procedure is as follows: (i) a certain volume of irrigation water is applied to a fraction of the tables (this volume is lower than the 500 m^3 ha^{-1} because only a fraction of the tables receives the 5-cm water layer), (ii) this water flows back to the mixing tank and is supplemented with water from the basin, (iii) the water in the mixing tank is applied to a next fraction of the tables. Another possiblity is that the water is applied to a fraction of the tables and then flows to the used-water tank, is disinfected and reused for a next fraction of the tables. Both options are logistically possible because the irrigation procedure takes only about 0.5 h and irrigation is needed every two or three days. Both options will, in case of spray and LVM applications, lead to higher concentrations in the used-water tank than calculated with a cultivation tank of 500 m^3 ha^{-1} because the same amount of pesticide deposited on the tables during application is taken up by a smaller water volume than 500 m^3 ha^{-1}. We consider the volume of 95 m^3 ha^{-1} of the cultivation tank to be a conservative estimate for mimicking these irrigation procedures. If more information on the actual volumes of the irrigation water and the irrigation procedure becomes available, we recommend to improve SEM-P by mimicking the actual irrigation procedures more closely.

4.3 Processes in the recirculation tanks

The conservation equations for the mass of parent substance and metabolite in all tanks except the cultivation tank are the same as for SEM-S:

$$\frac{dm_{pa,i}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,i} c_{w,j} - \sum_{j=1}^{\lambda} Q_{fl,i,j} c_{w,i} - V_{w,i}\, k_{t,pa,i}\, c_{w,i} + \dot{m}_A \qquad \text{Eqn 27}$$

$$\frac{dm_{me,i}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,i} C_{w,j} - \sum_{j=1}^{\lambda} Q_{fl,i,j} C_{w,i} - V_{w,i}\, k_{t,me,i}\, C_{w,i} + V_{w,i}\, \chi\, \frac{m_{mol,me}}{m_{mol,pa}}\, k_{t,pa,i}\, c_{w,i} \qquad \text{Eqn 28}$$

For the cultivation tank (i.e. the ebb/flood irrigation water), the processes differ. In this tank the uptake of the substances occurs by the pots (so not by the roots):

$$\frac{dm_{pa,tab}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,tab} c_{w,j} - \sum_{j=1}^{\lambda} Q_{fl,tab,j} c_{w,tab} - V_{w,tab}\, k_{t,pa,tab}\, c_{w,tab} - Q_{up,pots}\, c_{w,tab} + \dot{m}_A \qquad \text{Eqn 29}$$

$$\frac{dm_{me,tab}}{dt} = +\sum_{j=1}^{\nu} Q_{fl,j,tab} C_{w,j} - \sum_{j=1}^{\lambda} Q_{fl,tab,j} C_{w,tab} - V_{w,tab}\, k_{t,me,tab}\, C_{w,i} + V_{w,tab}\, \chi\, \frac{m_{mol,me}}{m_{mol,pa}}\, k_{t,pa,tab}\, c_{w,tab} - Q_{up.pots} C_{w,tab} \qquad \text{Eqn 30}$$

where the subscript ‘tab’ indicates the irrigation water on the tables (i.e. the cultivation tank) and $Q_{up,pots}$ is the volume rate of uptake of water by the pots (m^3 d^{-1}). Note that the TSCF does not play a role here because the uptake of water from the cultivation tank takes place by the pots driven by suction of the soil moisture in the pots during the 0.5-h irrigation event. This leads to a convective flow of the pesticide into the pots which is not influenced by the uptake of pesticide by the roots.

The above equations do not include an exchange flux between the cultivation water and the greenhouse air because the cultivation water is only in contact with the air during the irrigation events. Since formation of metabolites is assumed to occur only in recirculation water, they only occur there—this is the same procedure as in SEM-S.

The rate coefficients $k_{t,pa,i}$ and $k_{t,me,i}$ are temperature dependent which is described with the Arrhenius equation. For the disinfector tank it is furthermore an option to provide the fraction of the substance that is removed relative to the mass flowing through the tank, instead of the half-life. This form of removal is not corrected for temperature. The temperature of the cultivation and the drainage tanks is assumed to be equal to the air temperature in the greenhouse and that of the other tanks is assumed to be 2^{o}C colder because these other tanks are not located in the greenhouse.

The concentrations of substance (parent or metabolite) in each tank are simply calculated as the quotient of the mass in the tank and the volume of water in the tank. Note that no sorption is considered for crops grown into pots (see Boesten et al. (2019) for background information on the rationale behind not including sorption explicitly).

In case of application via the irrigation water (SEM-Pi), the dose is added to the mixing tank (Figure 5). The model assumes that the application of a pesticide is not instantaneous: it is assumed that an application takes 2 h. During each time step within the application period, an equivalent amount of pesticide is introduced.

Purification of wastewater is included using the same procedure as in SEM-S: by multiplying the concentrations that enter the surface water by a purification reduction factor.

The masses in the tanks were integrated using Euler's method of rectilinear integration (same procedure as in SEM-P).

4.4 Processes in greenhouse outside the recirculation water tanks

4.4.1 Main concepts

After spray or LVM applications, pesticide can contaminate the water in the tanks by deposition onto the tables during application, as well as via the condensation water. As in SEM-S, the condensation-water route is quite complicated as is illustrated by the scheme of Figure 9. After a pesticide application part of the dose is deposited on the plants, the soil in the pots, the roof and the tables (which are likely to be dry then). The deposits on the plants, the pots, the tables and the roof volatilise and thus contaminate the air in the greenhouse. The model includes also a flux for the deposition from the air to the pots in case the concentration in the gas phase at the surface of the pots is lower than in the air. The deposit on the roof may dissolve directly into the condensation water. The deposits on the plant and in the pots may also dissipate due to processes other than volatilisation (not shown in the scheme). Wash-off from the plants is not considered. The model includes exchange fluxes between the air in the greenhouse and the condensation water. Furthermore, pesticide disappears from the greenhouse into the outside air by ventilation.

The pesticide on the greenhouse floor is not included in SEM-P because the tables with the pots cover the surface area of the greenhouse to such a large extent that the deposition on the floor can be ignored. The deposition fraction is instead considered to end up on the tables and the pots.

As indicated by Figure 9, there are no fluxes from any tank to the greenhouse air so the metabolite is retained in the tanks and the remainder of this chapter deals with the parent substance.

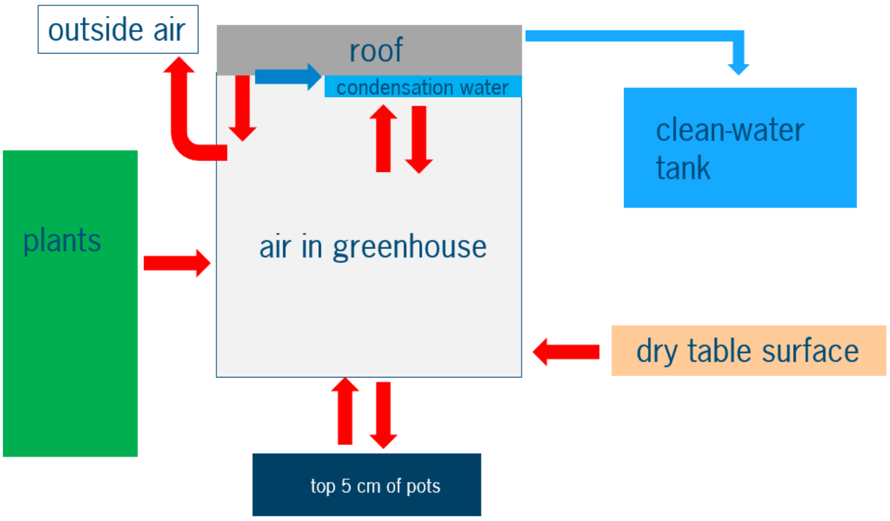

Figure 9 *Schematic representation of the processes related to the concentration in the air of the greenhouse in SEM-P. The condensation water is assumed to be present on the roof. The red arrows are gas fluxes of the substance and the blue arrows are water fluxes that carry substance.*

In line with Figure 9, the model includes simulation of the following quantities as a function of time:

- The mass of pesticide on the plants per surface area of greenhouse, A_p (kg m^{-2})
- The mass of pesticide in the greenhouse air per surface area of greenhouse, A_a (kg m^{-2})
- The mass of pesticide on the roof per surface area of greenhouse, A_r (kg m^{-2})
- The mass of pesticide in the condensation water on the greenhouse roof per surface area of greenhouse, $A_{w,cds}$ (kg m^{-2})
- The concentration in the greenhouse air, $c_{a,g}$ (kg m^{-3})
- The concentration in the condensation water on the roof, $c_{w,cds}$ (kg m^{-3})
- The mass of pesticide on the pots, A_{tab} (kg m^{-2})
- The mass on the tables per surface area of greenhouse, A_{tab} (kg m^{-2})

4.4.2 Distribution of dose after spray or LVM applications

During a spray application no pesticide is added to the air or the condensation water. So immediately after the first spray application, the air and condensation water are free of substance. It is assumed that 0.1% of the dose is deposited on the roof (so $f_r = 0.001$).

Immediately after an LVM application, the concentration in the air is equal to the concentration of a saturated vapour. No pesticide is added to the condensation water during an LVM application. It is assumed that 1% of the dose is deposited on the roof (so $f_r = 0.01$).

The rest of the applied dose is deposited on the pots and the tables. Again, application of pesticide is assumed to occur over a period of 2 hr. For LVM the air is assumed to be saturated first (see Eqn 10).

The distribution of the deposition between the pots and the tables is based on $f_{pot\text{-}area}$, i.e. the fraction of the surface area of the tables covered by the pots. $f_{pot\text{-}area}$ is 0.3 in the model. Hence, 30 percent of the fraction deposited on the pots and tables in deposited on the pots and 70 percent on the tables.

4.4.3 The pesticide fluxes in the gas phase

The fluxes $J_{v,p}$, J_{vent}, $J_{a/w}$ and $J_{v,r}$ in SEM-P are identical to those in SEM-S.

Because irrigation occurs as short events, it is likely that the tables are dry during application, and pesticide will not immediately enter the recirculation water. During the time between application and irrigation volatilisation from the dry tables may occur. Ignoring this process would result in overestimation of the concentration in the recirculation water, particularly for volatile substances. Therefore, we assume that the areic mass deposited on the tables volatilises during one day from a dry table surface, after which the remaining residue is dissolved in the irrigation water (i.e. in the cultivation tank). The reasoning behind using one day is that it is estimated that on average the frequency of the flooding of the tables is every two days, hence one day is considered a good estimate for the time between application and flooding.

This volatilisation flux is described by $J_{v,tab}$ (kg m^{-2} d^{-1}):

$$J_{v,tab} = \left(1 - f_{pot}\right) \frac{A_{tab}}{A_{tab,i}} \frac{c_{a,sat} - c_{a,g}}{r_{a,dt}} \qquad \text{Eqn 31}$$

where $A_{tab,i}$ is the initial value of A_{tab}, $r_{a,dt}$ is the resistance of the boundary layer of the dry table (set at 200 s m^{-1}). After this first day, the remaining residue is taken up by the irrigation water and there is no further volatilisation from or deposition onto the water until the next application (because the water is present in a tank). This procedure is different from that in the previous GEM version, which assumed that there was continuously a permanent water layer on the tables.

The gas fluxes for the exchange between the pots and the air are described by:

$$J_{d,pot} = f_{pot} \; \frac{c_{a,g} - c_{g,pot,sur}}{r_{a,pot}} \qquad \text{Eqn 32}$$

or

$$J_{v,pot} = f_{pot} \; \frac{c_{g,pot,sur} - c_{a,g}}{r_{a,pot}} \qquad \text{Eqn 33}$$

where $J_{d,pot}$ is the mass flux of pesticide (kg m^{-2} d^{-1}) from the air to the pots, $J_{v,pot}$ is the mass flux of pesticide (kg m^{-2} d^{-1}) from the pots to the air, $c_{g,pot,sur}$ is the concentration in the gas phase at the surface of the pots (kg m^{-3}), and $r_{a,pot}$ is the boundary layer resistance (d m^{-1}) at the pot surface (set at 200 s m^{-1}).

4.4.4 Sub-model for calculating the concentration in the gas phase at the surface of the pots

This $c_{g,pot,sur}$ is calculated by a sub-model that describes the pesticide behaviour in the top 5 cm of the pots. Pots are typically 15 cm high and receive about every two days irrigation by a water layer of about 5 cm that is put on the tables and which drains away in 15-20 min. So there is a periodic upward flow of water in the pots induced by the water uptake of the plant roots. We assume as a pragmatic approach that the water flow in the top 5 cm can be ignored and that in this top 5 cm only diffusion takes place (both in liquid and gas phase) and degradation. This is more or less the same approach as in earlier versions of GEM in which a 2-mm layer is considered in which only diffusion and degradation takes place.

The organic matter content in this top 5 cm is set at 10%, the dry bulk density at 1 kg dm^{-3}, the porosity at 0.6 and the volume fraction of liquid at 0.3.

The sub-model in this top 5 cm is based on the following conservation equation:

$$\frac{\partial c_{sys,pot}}{\partial t} = -\frac{\partial J_{dif,l}}{\partial z} - \frac{\partial J_{dif,g}}{\partial z} - k_{pot} c_{sys,pot} \qquad \text{Eqn 34}$$

where $c_{sys,pot}$ is the total concentration in soil, including gaseous, dissolved, and sorbed (kg m^{-3}), t is time (d), $J_{dif,l}$ is the diffusion flux (kg m^{-2} d^{-1}) in the liquid phase, z is depth in soil (m), $J_{dif,g}$ is the diffusion flux (kg m^{-2} d^{-1}) in the gas phase and k_{pot} is the degradation rate coefficient (d^{-1}).

The concentration in total soil is the sum of the amounts in the liquid and gas phase and the amount sorbed. Assuming a linear sorption isotherm and a sorption coefficient proportional to the organic matter content gives the following expression:

$$c_{sys,pot} = \varepsilon\ c_{g,pot} + \theta\ c_{l,pot} + \rho_{pot}\ m_{om}\ K_{om}\ c_{l,pot} \qquad \text{Eqn 35}$$

where ε is the volume fraction of gas in soil (-), $c_{g,pot}$ is the concentration in the gas phase in soil (kg m^{-3}), θ is the volume fraction of liquid in soil (-), $c_{l,pot}$ is the concentration in the liquid phase in soil (kg m^{-3}), ρ_{pot} is the dry bulk density of the soil in the pots (kg m^{-3}), m_{om} is the mass fraction of organic matter (-), and K_{om} is the organic-matter/water distribution coefficient (m^3 kg^{-1}).

The diffusion flux $J_{dif,l}$ is calculated as:

$$J_{dif,l} = -\ D_{dif,l} \frac{\partial c_{l,pot}}{\partial z} \qquad \text{Eqn 36}$$

where $D_{dif,l}$ is the diffusion coefficient in the liquid phase (m^2 d^{-1}). This diffusion coefficient is estimated using the Millington-Quirk approach used in the PEARL model (Van den Berg et al., 2016):

$$D_{dif,l} = \frac{\theta^2}{(\varepsilon+\theta)^{\frac{2}{3}}}\ D_{dif,w} \qquad \text{Eqn 37}$$

where $D_{dif,w}$ is the diffusion coefficient in water (m^2 d^{-1}). This gives for a porosity of 0.6 and a volume fraction of liquid of 0.3 a proportionality factor of 0.127.

The diffusion flux $J_{dif,g}$ is calculated as:

$$J_{dif,g} = -\ D_{dif,g} \frac{\partial c_{g,pot}}{\partial z} \qquad \text{Eqn 38}$$

where $D_{dif,g}$ is the diffusion coefficient in the gas phase (m^2 d^{-1}), also estimated using the Millington-Quirk approach (Van den Berg et al., 2016):

$$D_{dif,g} = \frac{\varepsilon^2}{(\varepsilon+\theta)^{\frac{2}{3}}}\ D_{dif,a} \qquad \text{Eqn 39}$$

where $D_{dif,a}$ is the diffusion coefficient in air (m^2 d^{-1}). This gives for a porosity of 0.6 and a volume fraction of liquid of 0.3 also a proportionality factor of 0.127.

The concentration in the gas is directly proportional to that in the liquid phases:

$$c_{g,pot} = K_H\ c_{l,pot} \qquad \text{Eqn 40}$$

where K_H is the Henry coefficient (-). Thus, the diffusion flux in the gas phase can be written in terms of the concentration in the liquid phase:

$$J_{dif,g} = -\ D_{dif,g}\ K_H \frac{\partial c_{l,pot}}{\partial z} \qquad \text{Eqn 41}$$

With help of this equation, the right hand side of the conservation equation can be simplified by considering only the concentration gradient of $c_{l,pot}$:

$$\frac{\partial c_{sys,pot}}{\partial t} = +\left(D_{dif,g}\ K_H + D_{dif,l}\right)\frac{\partial^2 c_{l,pot}}{\partial z^2} - k_{pot} c_{sys,pot} \qquad \text{Eqn 42}$$

The bottom boundary condition is a zero flux.

In case of a pesticide application, an areic mass A_{pot} is deposited on the pots; this is defined as the mass deposited on the pots per surface area of greenhouse (see Section 4.4.2). Then the following concentration $c_{sys,pot,app}$ (kg m^{-3}) has to be added to the system concentration in the first numerical compartment:

$$c_{sys,pot,app} = \frac{A_{pot}}{f_{pot}\ \Delta z_{top}} \qquad \text{Eqn 43}$$

where Δz_{top} is the thickness of the top numerical compartment. It is necessary to divide by f_{pot} in this equation because A_{pot} is defined per surface area of greenhouse and only a fraction f_{pot} of this surface area is covered by the pots.

The conservation equation is solved using finite difference approximations similar to those of the PEARL model (Van den Berg et al., 2016). The soil is divided into numerical compartments and at the top the approximations generate the concentration at a depth of 0.5 × Δz_{top}. However, the flux to or from the air in the greenhouse has to be based on the concentration at the soil surface ($c_{g,pot,sur}$, see the equations for the gas flux between the soil and the air). This $c_{g,pot,sur}$ can be calculated by requiring that the gas flux between the soil surface and the air is equal to the diffusion flux out of the top compartment:

$$\frac{c_{a,g} - c_{g,pot,sur}}{r_{a,pot}} = -\left(D_{dif,g}\ K_H + D_{dif,l}\right)\frac{c_{l,pot,top} - c_{l,pot,sur}}{0.5 \times \Delta z_{top}} \qquad \text{Eqn 44}$$

where $c_{l,pot,sur}$ is the concentration in the liquid phase at the soil surface (kg m^{-3}) which is equal to $K_H \times c_{g,pot,sur}$. It can then be shown that

$$c_{g,pot,sur} = K_H \frac{r_s\ c_{a,g} + r_{a,pot}\ c_{l,pot,top}}{r_{a,pot} + K_H\ r_s} \qquad \text{Eqn 45}$$

with

$$r_s = \frac{0.5 \times \Delta z_{top}}{D_{dif,g}\ K_H + D_{dif,l}} \qquad \text{Eqn 46}$$

Substituting this result into the left-hand side of Eqn 44 gives the following result for the diffusion flux ($J_{dif,sur}$) at the soil surface:

$$J_{dif,sur} = \frac{c_{a,g} - K_H\ c_{l,pot,top}}{r_{a,pot} + K_H\ r_s} \qquad \text{Eqn 47}$$

Based on the numerical analysis of the PEARL model (Van den Berg et al., 2016), the maximum time step for the submodel of this top 5 cm can be approximated by

$$\Delta t \quad \leq \quad \frac{\frac{1}{2}\Delta z^2\left(\varepsilon K_H + \theta + \rho_{pot} m_{om} K_{om}\right)}{D_{dif,l} + K_H\ D_{dif,g}} \qquad \text{Eqn 48}$$

where Δt is this maximum time step (d) and Δz is the thickness of the numerical compartments (m). We suggest to use 1-mm thick compartments as this should give for most pesticides a reasonable accuracy for the concentration profile in the top 5 cm. Using the parameters described above, K_{om} = 0, $D_{dif,w}$ = 0.4 × 10^{-4} m^2 d^{-1} and $D_{dif,a}$ = 0.4 m^2 d^{-1} gives for Δz = 1 mm and for K_H = 10^{-4} a maximum time step of 0.03 d. The current time step of GEM is about 10^{-3} d, so it is unlikely that this submodel will lead to the need of using a smaller time step in GEM.

In Annex 9 an analysis is done on the penetration depth into the pots, which showed that the penetration depths is likely to be limited to 5 cm.

4.4.5 The pesticide fluxes in the water phase

The mass flux for the dissolution of pesticide deposited onto the roof, J_{dis}, and mass flux of pesticide from the pool of condensation water to the clean-water tank, J_{cds}, are identical to those in SEM-S (see also Eqns 18 and 19, respectively). The rate equations for amounts on plants, roof and in air and condensation water

The rate equations for A_p, A_r and $A_{w,cds}$ are identical to those for SEM-S.

The rate equation for A_a is given by:

$$\frac{dA_a}{dt} = J_{a/w} + J_{v,p} + J_{v,pot} - J_{d,pot} + J_{v,r} - J_{vent} \qquad \text{Eqn 49}$$

The numerical solution of the rate equations consist of Euler's method so assuming that the rates are constant during the integration interval. The time step is fixed to 1 min. The explicit scheme has the consequence that it may lead to negative values of the quantity that is integrated. This was prevented using the iteration procedure of Annex 6 as described before for SEM-S.

4.5 Expected effects of changes in SEM-P

As described before, the water regime in SEM-P was changed considerably. The previous version assumed a permanent water layer on the tables whereas the revised version assumes that the tables are dry for most of the time and that irrigation water is only present on the tables for about half an hour every 2 or 3 days[9]. In the previous version, there is continuously an exchange flux between this water layer and the greenhouse air whereas in the revised version there is volatilisation from the dry table during the first day after application, after which the pesticide is taken up by the irrigation water and no further volatilisation occurs because the irrigation water is present in a tank.

For applications to the irrigation water is a new application option for pots on tables in GEM, therefore the impact on the calculated concentrations is unknown. The probable effects of the change for spray applications were assessed using a simplified version of the SEM-P model as described in Annex 8. This assessment was based on old values for the distributions of the dose over plants, pots and tables (old 87-4-9% and new 39-18-42%, respectively) but we expect that the conclusions with respect to the effect of the water regime will not change. The conclusions of this exercise were:

for pesticides with saturated vapour pressures below 10^{-5} Pa the change in the water regime has probably no effect on the emissions because volatilisation processes are insignificant for both water regimes

the change of the water regime will probably lead to lower emissions for pesticides with water solubilities above 1 mg/L and saturated vapour pressures above 10^{-5} Pa (because of low volatilisation rates from the permanent water layer on the tables and thus high emission concentrations for the previous version)

for pesticides with water solubilities below 1 mg/L and saturated vapour pressures above 10^{-5} Pa, the change in the water regime will probably lead to higher emissions but such pesticides do not occur in the list of most frequently used pesticides in crops grown on tables provided by Wipfler et al. (2015).

These conclusions are probably also valid for LVM applications because differences between the calculation procedures for spray and LVM applications are relatively small. We recommend to check these conclusions by calculations with the complete model.

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[9] This holds for the fate processes, the water flows are considered to be continuous.

Other main changes in the model are:

1. The amounts of pesticide in the air plus the condensation water immediately after a spray or LVM application have been strongly reduced (from 8% to 0% for spray and from 35% to about <1% for LVM applications leading to decreased emission concentrations),
2. The concentration in the air at the plant surface after spray or LVM applications has been reduced from 100% to 20% of the saturated vapour concentration (leading to decreased emission concentrations),
3. The sorption equilibrium between the bottom 10 cm of the pots and the water on the tables has been removed (leading to increased emission concentrations),
4. For spray or LVM applications, deposition of 0.1-1% of the dose on the roof has been added (leading to increased emission concentrations)
5. For spray of LVM applications, about 40% of the dose is deposited on the tables, about 20% on the pots and about 40% on the plants compared to about 10% on tables, 5% on pots and 85% on plants in previous version[10] (leading to increased emission concentrations because of the increased deposition on the tables)
6. The submodel of the pots that describes the behaviour of the pesticide deposited on the pot surface includes also diffusion in liquid phase (a priori unknown direction of effect on emission concentrations).

Let us consider the effect of removing the sorption equilibrium between the bottom 10 cm of the pots and the water on the tables. The previous SEM-P assumed a water volume in the cultivation tank of 125 m^3 per ha. Both the current and previous SEM-P assume a dry bulk density of the pots of 1000 kg m^{-3}, an organic matter content of 10% and a fraction of the pot surface area of 0.3. So considering 1 m^2 of greenhouse gives then 12.5 L of water which is in sorption equilibrium with 0.10×0.10 m $\times$ 1000 kg $m^{-3} \times 1$ $m^2 \times 0.3 = 3$ kg of organic matter. The decrease in the concentration in the cultivation tank due to the sorption equilibration equals then a factor of $12.5/(12.5 + 3\ K_{om})$. The K_{om} of the seven pesticides used by Wipfler et al. (2015) for their impact assessment of the previous SEM-P ranged between 3 and 18 000 L/kg with a median of 129 L/kg. This gives a range of this factor between 0.0002 to 0.6 (0.03 for the median K_{om}). So for most of the pesticides, removing the sorption equilibrium increases the concentration in the cultivation tank by at least a factor of 30.

Overall, we expect that the revised SEM-P generates for most cases higher emission concentrations than the previous version because the sorption equilibrium between the bottom 10 cm of the pots and the water on the tables has been removed and because the deposition on the tables has increased from about 10 to 40%. This expectation needs confirmation by calculations with the SEM-P model.

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[10] For very young plants numbers are different.

5 Discussion

5.1 Instantaneous dissolution for SEM-S

The most straightforward approach for A_s (deposition on the slabs) and A_t (deposition on the troughs) is to add these to the cultivation and drainage tanks. This is also implemented in GEM4.

However the pesticide has to dissolve into the recirculation water. The volume of water in part A of the cultivation tank in SEM-S is 47 m^3 ha^{-1} (Figure 5). Let us consider a pesticide application of 1 kg/ha. This leads to A_s = 0.01 kg ha^{-1} which corresponds with a concentration in the water of 0.2 mg/L. This is based on perfect mixing of the part-A tank and no sorption. We can also look at this problem from the point of view of the water flow: in spring 3 mm/d is typical evapotranspiration rate which corresponds with a water flow rate entering the tank of 30 m^3/d. Dissolving 0.01 kg ha^{-1} in 30 m^3 gives a concentration of 0.3 mg/L.

Wipfler et al. (2015) selected frequently used pesticides that are currently applied by spray or LVM in Dutch crops grown on slabs. Their $c_{w,sol}$ values shown in Figure 10 indicate that one-third of the in total 18 substances have a $c_{w,sol}$ below about 0.5 mg/L and that two-third of these pesticides have water solubilities that are considerably higher than 0.2-0.3 mg/L. For the dissolution of the deposit on the troughs this situation is similar: the deposited fraction is only 0.003, so three times lower than for the mats but also water flow rates are a factor two to three lower.

To solve this issue the dissolution flux of A_s and A_t could be included in the model. The most simple approach would be assuming that the dissolution flux is described by:

$$J_{dis,culA} = q_{culA}\left(c_{w,sol} - c_{w,mix}\right) \qquad \text{Eqn 50}$$

$$J_{dis,dra} = q_{dra}\left(c_{w,sol} - c_{w,culB}\right) \qquad \text{Eqn 51}$$

where $J_{dis,culA}$ is an additional flux of substance flowing into the part-A cultivation tank (kg m^{-2} d^{-1}), q_{culA} is the water flow rate per surface area of greenhouse into the part-A cultivation tank (m d^{-1}), $c_{w,mix}$ is the concentration in the water flowing out of the mixing tank (kg m^{-3}), where $J_{dis,dra}$ is an additional flux of substance flowing into the drainwater tank, q_{dra} is the water flow rate per surface area of greenhouse into the drainwater tank (m d^{-1}) and $c_{w,culB}$ is the concentration in the water flowing out of the part-B cultivation tank. These substance fluxes are valid until A_s or A_t become zero. In the exceptional cases that $c_{w,mix}$ or $c_{w,culB}$ exceed $c_{w,aol}$ the fluxes are set to zero as well. Please note that these $J_{dis,culA}$ and $J_{dis,dra}$ still have to be multiplied with the surface area of the greenhouse when included in Eqn 1 because this equation considers the rate change of the total mass in the greenhouse. Furthermore it should be kept in mind that the proposed approach is also a conservative approach, i.e. 'on the safe side' because it assumes that the concentrations in the water flows equal the water solubility (i.e. the maximum possible concentration).

We recommend to include the proposed approach outlined above in future versions of GEM.

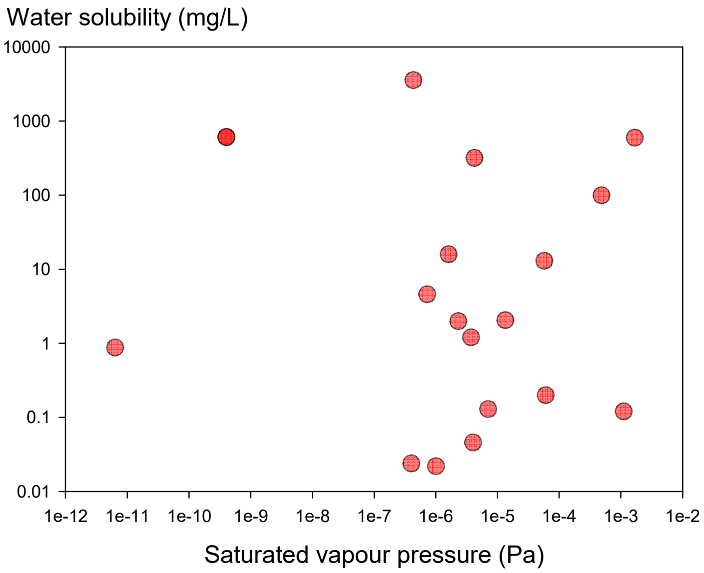

Figure 10 *Water solubility as a function of saturated vapour pressure for the pesticides selected by Wipfler et al. (2015) for SEM-S calculations.*

5.2 Instantaneous dissolution on the tables

For the water on the tables it is assumed that the deposit on the tables is instantaneously dissolved in the irrigation water. For pesticides that are not volatile, the deposit on the tables will be 41-42% of the dose (see Section 4.4.2). Let us consider a dose of 1 kg/ha: dissolving 0.4 kg in a volume of 95 m^3 gives a concentration of 4 mg/L. Wipfler et al. (2015) selected the most important pesticides that are currently applied by spray or LVM applications to pot plants in Dutch greenhouses. Figure 11 shows that three out of the seven selected pesticides had a water solubility less than 4 mg/L. So it is a point of debate whether the dissolution in the irrigation water should be included in the model. We decided not to do so because this would lead to further complications: it would become necessary to include also volatilisation of the deposit on the tables after the first irrigation event (see start of Section 4.4.3). We recommend to improve this aspect once more information has become available on the irrigation procedures for crops grown in pots.

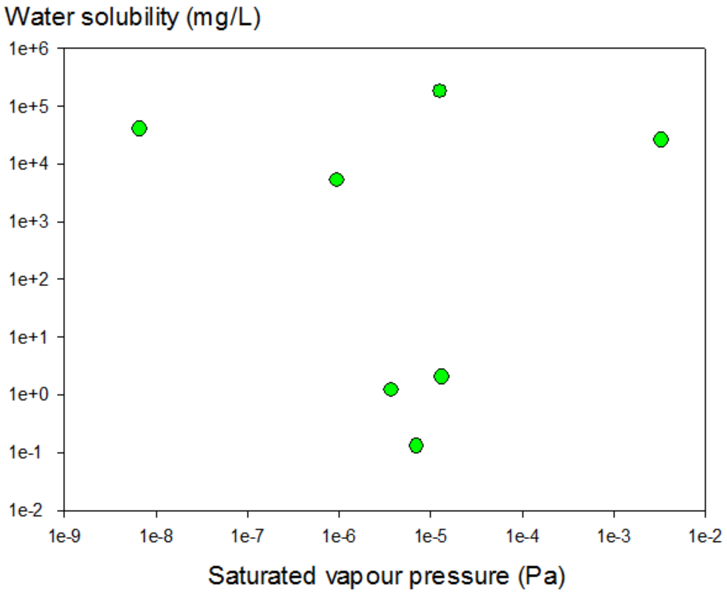

Figure 11 *Water solubility as a function of saturated vapour pressure for the pesticides selected by Wipfler et al. (2015) for SEM-P calculations.*

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Annex 1 List of symbols

Symbol	Quantity	Unit
a	parameter in relationships for describing the fraction of the dose that is deposited on pots, tables and plants in SEM-P	-
b	parameter describing the increase of the available leaf area surface in case application occurs both on top and underside of the leaves	-
$c_{a,g}$	mass concentration of pesticide in greenhouse air	kg m^{-3}
$c_{a,sat}$	mass concentration of pesticide in air corresponding with saturated vapour pressure (saturated vapour concentration)	kg m^{-3}
$c_{a,tab}$	mass concentration of pesticide in air at surface of dry tables	kg m^{-3}
$c_{g,pot}$	mass concentration in the gas phase in soil	kg m^{-3}
$c_{g,pot,sur}$	mass concentration of pesticide in air at surface of the pots	kg m^{-3}
$c_{l,pot}$	mass concentration in the liquid phase in soil	kg m^{-3}
$c_{sys,pot}$	concentration in the soil system of the pots	kg m^{-3}
$c_{w,cds}$	mass concentration of pesticide in condensation water	kg m^{-3}
$c_{w,i}$	mass concentration of parent substance in water of tank *i*	kg m^{-3}
$c_{w,tab}$	mass concentration of pesticide in irrigation water on the tables	kg m^{-3}
$c_{w,sol}$	mass concentration of pesticide at water solubility	kg m^{-3}
$c_{w,sol,ref}$	mass concentration of pesticide at water solubility for reference temperature	kg m^{-3}
f_a	fraction of dose in the air immediately after application	-
f_{con}	fraction of floor surface that is contaminated with spray or LVM deposits	-
f_f	fraction of dose deposited on floor	-
f_{foil}	factor for incomplete contact between foil and water in slabs	-
f_p	fraction of dose applied to plants	-
f_{pot}	fraction of surface area that is covered with pots	-
$f_{pot+tab}$	fraction of the dose deposited on pots plus tables	-
f_r	fraction of dose deposited on roof	-
f_{sl}	fraction of dose dripped into slabs	-
f_{tr}	fraction of dose deposited on troughs that transport drainage water	-
g	proportionality factor to account for fact that only a small fraction of roof is covered by a deposit	-
k_f	rate coefficient for degradation of pesticide on floor	d^{-1}
k_p	rate coefficient for degradation of pesticide on plants	d^{-1}
k_{pot}	rate coefficient for degradation in pots	d^{-1}
$k_{t,me,i}$	rate coefficient of transformation of metabolite in tank *i*	d^{-1}
$k_{t,pa,i}$	rate coefficient of transformation of parent substance in tank *i*	d^{-1}
$k_{w,cds}$	rate coefficient for degradation in condensation water	d^{-1}
$m_{me,i}$	mass of metabolite in tank *i*	kg
m_{mol}	molar mass	kg mol^{-1}
$m_{mol,me}$	molar mass of metabolite	kg mol^{-1}
$m_{mol,pa}$	molar mass of parent	kg mol^{-1}
m_{om}	mass fraction of organic matter in pots	-
$m_{pa,i}$	mass of parent substance in tank *i*	kg
$m_{pa,tab}$	mass of parent substance in the irrigation water on the tables	kg
p	mass of tube divided by length of tube	kg m^{-1}
q_{cds}	volume flux of condensation water per surface area of greenhouse	m^{3} m^{-2} d^{-1}
q_{culA}	water flow rate per surface area of greenhouse into the part-A cultivation tank	m^{3} m^{-2} d^{-1}
q_{dra}	water flow rate per surface area of greenhouse into the drainwater tank	m^{3} m^{-2} d^{-1}
$r_{a,dt}$	boundary layer resistance for dry table	d m^{-1}

$r_{a,f}$	boundary layer resistance for floor	d m^{-1}
$r_{a,p}$	boundary layer resistance for plants	d m^{-1}
$r_{a,pot}$	boundary layer resistance for pots	d m^{-1}
$r_{a,r}$	boundary layer resistance for roof	d m^{-1}
$r_{a,w,cds}$	boundary layer resistance for condensation water	d m^{-1}
$r_{a,w,tab}$	boundary layer resistance for irrigation water on tables	d m^{-1}
t	time	d
z	depth in soil	m

A_a	mass of pesticide in air per surface area of greenhouse	kg m^{-2}
$A_{a,i}$	mass of pesticide initially in air per surface area of greenhouse	kg m^{-2}
A_f	mass of pesticide on floor per surface area of greenhouse	kg m^{-2}
$A_{f,i}$	mass of pesticide deposited on floor per surface area of greenhouse	kg m^{-2}
A_i	mass of pesticide applied per surface area of greenhouse	kg m^{-2}
A_p	mass of pesticide on plants per surface area of greenhouse	kg m^{-2}
$A_{p,i}$	mass of pesticide applied to plants per surface area of greenhouse	kg m^{-2}
A_{pot}	mass of pesticide in the pots per surface area of greenhouse	kg m^{-2}
$A_{pot,i}$	mass of pesticide deposited on the pots per surface area of greenhouse	kg m^{-2}
$A_{pot+tab,i}$	mass of pesticide per surface area of greenhouse deposited on pots plus tables	kg m^{-2}
A_r	mass of pesticide per surface area of greenhouse on roof	kg m^{-2}
$A_{r,i}$	mass of pesticide per surface area of greenhouse initially deposited on roof	kg m^{-2}
A_s	mass of pesticide per surface area of greenhouse dripped into slabs	kg m^{-2}
A_t	mass of pesticide per surface area of greenhouse on troughs	kg m^{-2}
$A_{tab,i}$	mass of pesticide initially deposited on tables per surface area of greenhouse	kg m^{-2}
$A_{w,cds}$	mass of pesticide in condensation water per surface area of greenhouse	kg m^{-2}
$C_{w,i}$	mass concentration of metabolite in water of tank *i*	kg m^{-3}
$D_{dif,a}$	diffusion coefficient in air	m^2 d^{-1}
$D_{dif,g}$	diffusion coefficient in the gas phase	m^2 d^{-1}
$D_{dif,l}$	diffusion coefficient in the liquid phase	m^2 d^{-1}
$D_{dif,w}$	diffusion coefficient in water	m^2 d^{-1}
D_{eff}	effective overall diffusion coefficient in pots	m^2 d^{-1}
E_v	molar enthalpy of vaporisation	J mol^{-1}
E_d	molar enthalpy of dissolution	J mol^{-1}
F	factor for decrease of pesticide concentration in gas phase at plant surface	-
GAI	Glass Area Index, i.e. surface area of roof divided by surface area of greenhouse	-
H_a	volume of air per surface area of greenhouse (so height of greenhouse)	m^3 m^{-2}
$H_{w,cds}$	volume of condensation water per surface area of greenhouse	m^3 m^{-2}
$H_{w,cir}$	volume of circulation water per surface area of greenhouse	m^3 m^{-2}
$J_{a/w}$	mass flux for exchange of pesticide between water on roof and air in greenhouse	kg m^{-2} d^{-1}
J_{cds}	mass flux of pesticide from condensation water to clean-water tank	kg m^{-2} d^{-1}
$J_{d,pot}$	mass flux of pesticide deposition onto pots	kg m^{-2} d^{-1}
$J_{d,tab}$	mass flux of pesticide deposition onto water on tables	kg m^{-2} d^{-1}
$J_{dif,l}$	mass flux due to diffusion in liquid phase in pots	kg m^{-2} d^{-1}
$J_{dif,g}$	mass flux due to diffusion in gas phase in pots	kg m^{-2} d^{-1}
$J_{dis,r}$	mass flux of dissolution of pesticide on roof surface	kg m^{-2} d^{-1}
$J_{dis,culA}$	mass flux of dissolution of pesticide flowing into the part-A cultivation tank	kg m^{-2} d^{-1}
$J_{dis,dra}$	mass flux of dissolution of pesticide flowing into drainwater tank	kg m^{-2} d^{-1}
$J_{v,f}$	mass flux of pesticide volatilisation from floor	kg m^{-2} d^{-1}
$J_{v,p}$	mass flux of pesticide volatilisation from plants	kg m^{-2} d^{-1}

$J_{v,pot}$	mass flux of pesticide volatilisation from pots	kg m^{-2} d^{-1}
$J_{v,r}$	mass flux of pesticide volatilisation rate from deposit on roof	kg m^{-2} d^{-1}
$J_{v,tab}$	mass flux of pesticide volatilisation from deposit on tables	kg m^{-2} d^{-1}
J_{vent}	mass flux of pesticide leaving the greenhouse by ventilation	kg m^{-2} d^{-1}
K_{foil}	linear sorption coefficient for sorption of pesticide to foil	m^{3} kg^{-1}
K_{H}	air-water partitioning coefficient (Henry coefficient)	-
K_{om}	organic-matter/water distribution coefficient	m^{3} kg^{-1}
K_{ow}	octanol-water partitioning coefficient	-
K_{sub}	linear sorption coefficient for sorption of pesticide to substrate	m^{3} kg^{-1}
K_{tube}	linear sorption coefficient for sorption of pesticide to a class of tubes/pipes	m^{3} kg^{-1}
L	length of class of tubes/pipes	m
LAI	Leaf Area Index	-
M_{foil}	mass of foil	kg
M_{roots}	mass of wet roots	kg
M_{sub}	mass of dry substrate (e.g. stonewool)	kg
N_{vent}	ventilation rate coefficient	d^{-1}
P_{sat}	saturated vapour pressure of pesticide	Pa
$P_{sat,ref}$	saturated vapour pressure of pesticide at reference temperature	Pa
$Q_{fl,j,i}$	volume rate of water flow from tank *j* to tank *i*	m^{3} d^{-1}
$Q_{fl,j,tab}$	volume rate of water flow from tank *j* to the water on the tables	m^{3} d^{-1}
$Q_{up,i}$	volume rate of uptake of water by plant roots from tank *i*	m^{3} d^{-1}
$Q_{up,pots}$	volume rate of uptake of water by the pots during irrigation events	m^{3} d^{-1}
$Q_{fl,ww}$	volume rate of water flow from the wastewater tank to the surface water	m^{3} d^{-1}
R	gas constant	J mol^{-1} K^{-1}
RCF	root concentration factor	m^{3} kg^{-1}
S_{gh}	surface area of greenhouse	m^{2}
S_{pec}	inner surface area of polyethene capillary tubes	m^{2}
S_{pei}	inner surface area of polyethene irrigation tubes	m^{2}
S_{PVC}	inner surface area of PVC transport pipe	m^{2}
T	greenhouse air temperature	K
T_{ref}	reference temperature	K
$TSCF_{me}$	transpiration stream concentration factor of metabolite	-
$TSCF_{pa}$	transpiration stream concentration factor of parent	-
$V_{w,i}$	volume of water in tank *i*	m^{3}
$V_{w,tab}$	volume of water on the tables	m^{3}
$V_{w,sub}$	volume of water in the cultivation tank	m^{3}
α	proportionality factor describing the efficiency of dissolution of pesticide deposited on roof surface in condensation water	-
ε	volume fraction of gas in pots	-
θ	volume fraction of water in pots	-
λ	number of outgoing water fluxes	-
ν	number of incoming water fluxes	-
ρ_{pot}	mass of dry soil per volume of soil in pots	kg m^{-3}
φ	purification reduction factor applied to concentration in wastewater tank	-
χ	molar fraction of parent that is transformed into metabolite	-
Δz_{top}	thickness of the top numerical compartment	m

Annex 2 Setpoints for filter rinsing water and sodium concentration in irrigation water to achieve discharge limits

Filter rinsing with 1.63 m^3 at each X m^3.

Period	Discharge				Reuse			
	Sweet pepper	Potplant (ficus)	Tomato	Rose	Sweet pepper	Potplant (ficus)	Tomato	Rose
2012-2014	9.5	13.5	20	13	20	20	20	20
2015-2017	19	27	42	100	20	20	20	20
2018-2020	70	65	85	100	20	20	20	100
2021-2024	21.5	90	46.5	33.5	20	20	20	20
2025-2027	45	75	100	68	20	20	20	20

Sodium concentration in supply water (mmol/l).

Period	Discharge				Reuse			
	Sweet pepper	Potplant (ficus)	Tomato	Rose	Sweet pepper	Potplant (ficus)	Tomato	Rose
default	50	50	50	50				
2012-2014	0.5	0.5	0.5	0.5	0.8	1	0.75	0.75
2015-2017	0.5	0.5	0.5	0.5	0.65	0.75	0.6	0.5
2018-2020	0.5	0.5	0.5	0.35	0.5	0.6	0.5	0.5
2021-2024	0.1	0.35	0.1	0.1	0.4	0.45	0.45	0.3
2025-2027	0.1	0.1	0.1	0.1	0.3	0.3	0.35	0.15

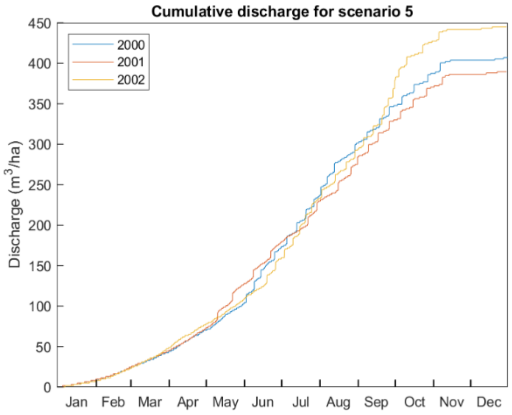
Annex 3 WaterStreams Model (WSM) parameters, version V2.0

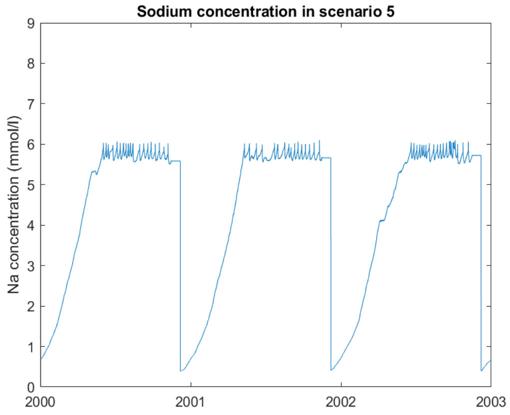
Parameter	Unit	Tomato	Sweet pepper	Rose	Ficus
Administrator					
Radiation factor		1.8	1.8	1.8	1.8
Heating factor		0.18	0.18	1	0.18
NO3 concentration in drain	mmol/l	30	22	16	12
N conc. in drain	g/l = kg/m^3	0.42	0.42	0.42	0.42
NH4 Recipe	mmol/l	0.1	0.5	0.1	0.1
NH4 Uptake	mmol/l	1	1	1	1
NO3 Recipe	mmol/l	10.75	12.5	11.25	10.5
NO3 Uptake	mmol/l	10.5	9.7	5.5	9.7
K Recipe	mmol/l	6.5	6.5	6.5	6.5
K Uptake	mmol/l	6.1	6.1	6.1	6.1
Na Recipe	mmol/l	0	0	0	0
Na conc based Uptake	mmol/l	0.06	0.01	0.001	0.01
Cl Recipe	mmol/l	0.75	1	0.75	0.75
Cl conc based Uptake	mmol/l	0.16	0.062	0.012	0.194
P Recipe	mmol/l	1.25	1.25	1.25	1.25
P vol. based Uptake	mmol/l	1.15	1.15	1.15	1.15
Ca Recipe	mmol/l	2.75	3.5	2.75	2.75
Ca vol. based Uptake	mmol/l	2.5	2.5	2.5	2.5
Mg Recipe	mmol/l	1	1.125	1	1
Mg vol. based Uptake	mmol/l	1	1	1	1
SO4 Recipe	mmol/l	1.5	1.5	1.5	1.5
SO4 vol. based Uptake	mmol/l	1.45	1.45	1.45	1.45
HCO3 Recipe	mmol/l	0	0	0	0
HCO3 vol. based Uptake	mmol/l	0	0	0	0
Fe Recipe	mmol/l	15E-3	15E-3	15E-3	15E-3
Fe vol. based Uptake	mmol/l	0	0	0	0
MN Recipe	mmol/l	10E-3	10E-3	10E-3	10E-3
Mn vol. based Uptake	mmol/l	0	0	0	0
Zn Recipe	mmol/l	4E-3	4E-3	4E-3	4E-3
Zn vol. based Uptake	mmol/l	0	0	0	0
B Recipe	mmol/l	20E-3	20E-3	20E-3	20E-3
B vol. based Uptake	mmol/l	0	0	0	0
Cu Recipe	mmol/l	0.75E-3	0.75E-3	0.75E-3	0.75E-3
Cu vol. based Uptake	mmol/l	0	0	0	0
N-norm 2017	kg N/ha	83	133	167	100
N-norm 2018-2021	kg N/ha	67	100	125	75
EC setpoint	mS/cm	3.7	2.7	2	1.7
Evaporation					
Evaporation model		De graaf	De graaf	De graaf	De graaf
LAI start		1.2	1.2	3	1.0
LAI max		3	3	3	2
Cultivation period begin	Day no	350	340	1	1
Cultivation period end	Day no	335	320	365	365
Greenhouse area	ha	1	1	1	1
Span width	m	4	4	4	4
Transmission cover	%	80	80	80	80
Heat buffer vol.	m^3/ha	300	300	300	300
Energy screen		yes	yes	yes	yes
Par transmission	%	76	76	76	76
NIR transmission	%	80	80	80	80
Insulation factor		0.45	0.45	0.45	0.45

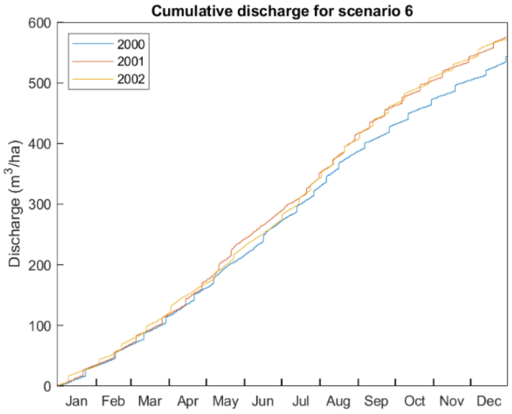
Annex 4 Detailed outcomes of the WaterStreams Model

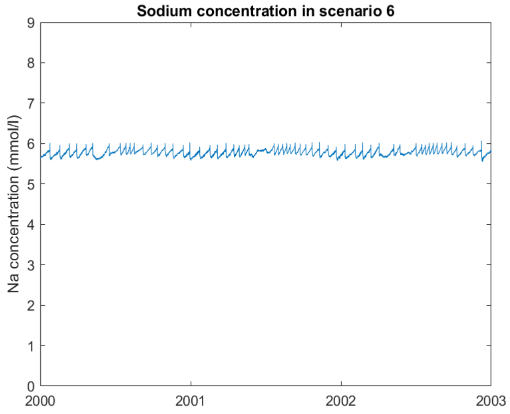
Scenario number

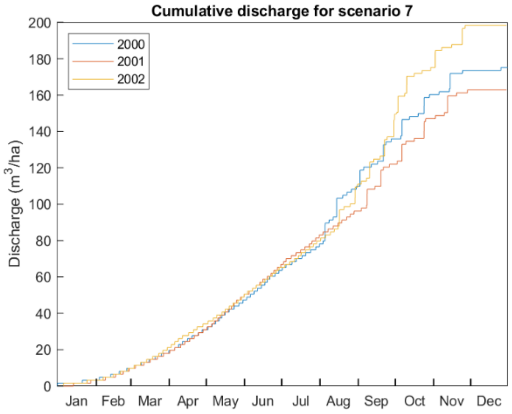
Period	Discharge				Reuse			
	Sweet pepper	Potplant (ficus)	Tomato	Rose	Sweet pepper	Potplant (ficus)	Tomato	Rose
2012-2014	1	2	3	4	21	22	23	24
2015-2017	5	6	7	8	25	26	27	28
2018-2020	9	10	11	12	29	30	31	32
2021-2024	13	14	15	16	33	34	35	36
2025-2027	17	18	19	20	37	38	39	40

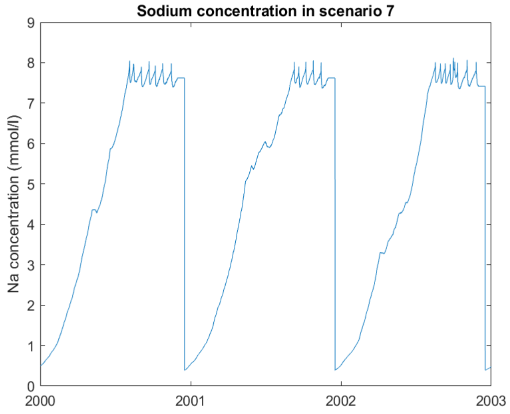

Cumulative discharge for scenario 5
Discharge (m^3/ha)
0
50
100
150
200
250
300
350
400
450
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec
2000
2001
2002

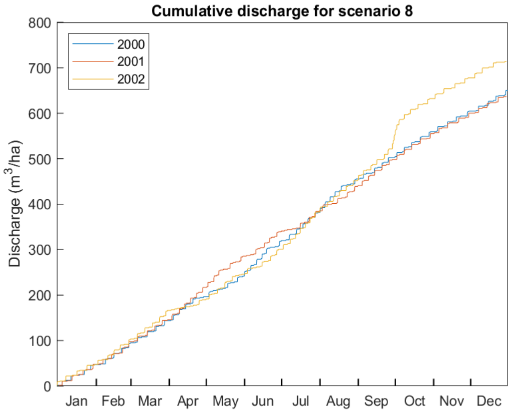

Sodium concentration in scenario 5
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

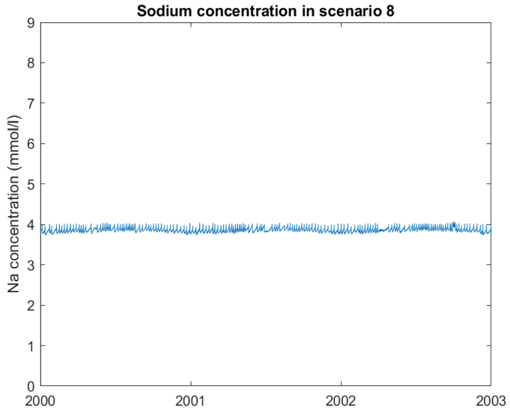

Cumulative discharge for scenario 6
Discharge (m^3/ha)
0
100
200
300
400
500
600
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec
2000
2001
2002

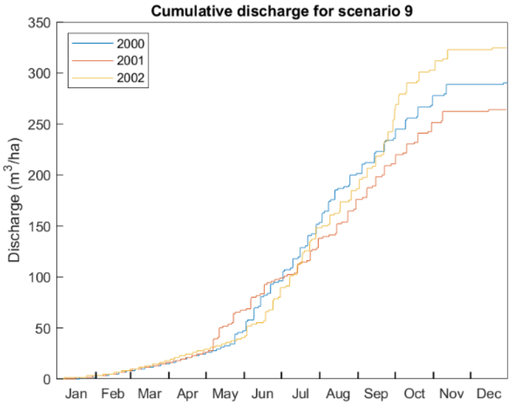

Sodium concentration in scenario 6
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

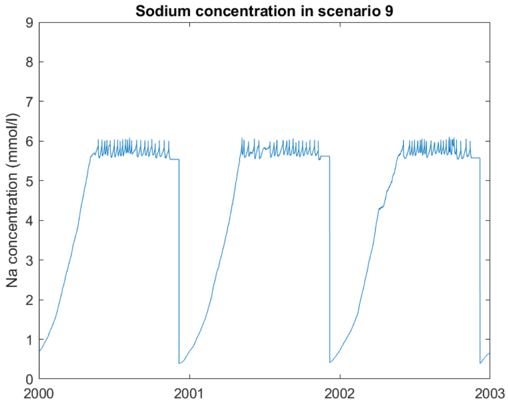

Cumulative discharge for scenario 7
Discharge (m^3/ha)
0
20
40
60
80
100
120
140
160
180
200
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec
2000
2001
2002

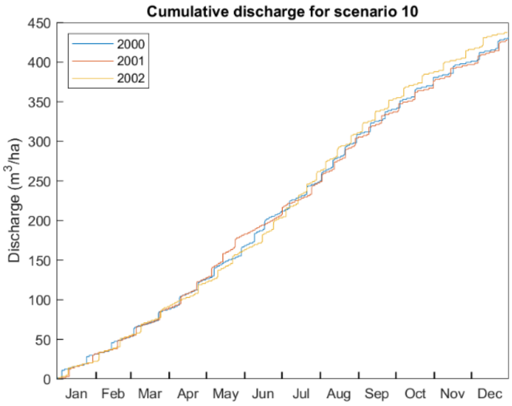

Sodium concentration in scenario 7
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

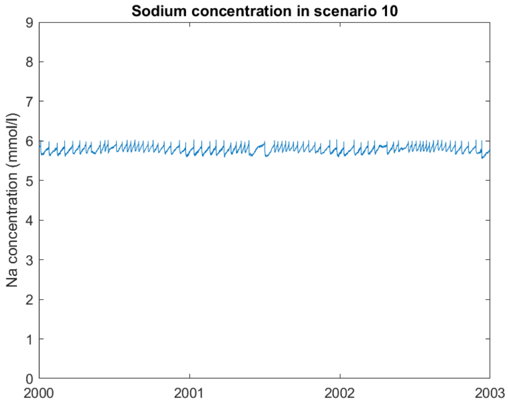

Cumulative discharge for scenario 8
Discharge (m^3/ha)
0
100
200
300
400
500
600
700
800
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec
2000
2001
2002

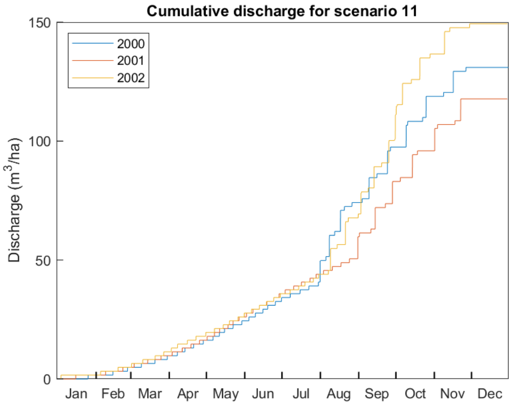

Sodium concentration in scenario 8
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

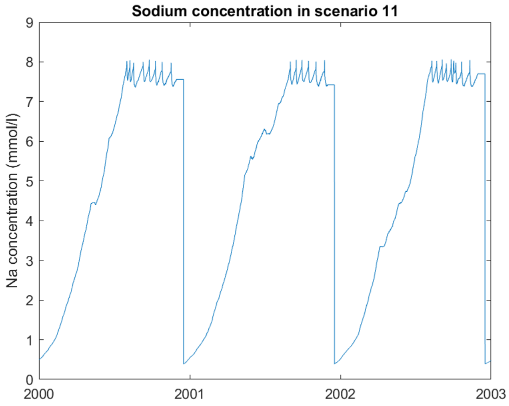

Cumulative discharge for scenario 9
Discharge (m³/ha)
350
300
250
200
150
100
50
0
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

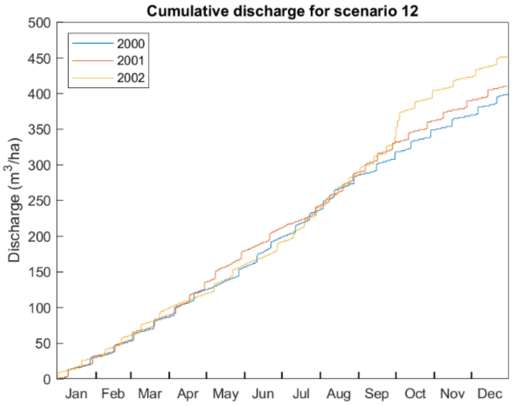

Sodium concentration in scenario 9
Na concentration (mmol/l)
9
8
7
6
5
4
3
2
1
0
2000
2001
2002
2003

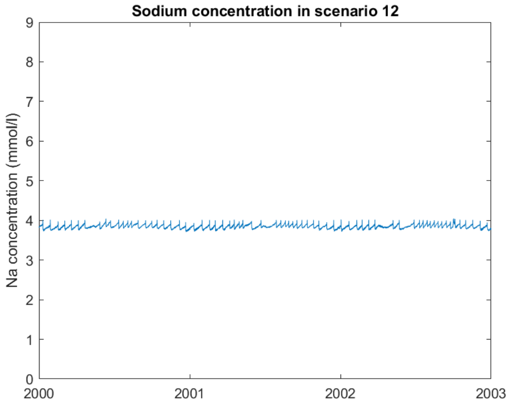

Cumulative discharge for scenario 10
Discharge (m³/ha)
450
400
350
300
250
200
150
100
50
0
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

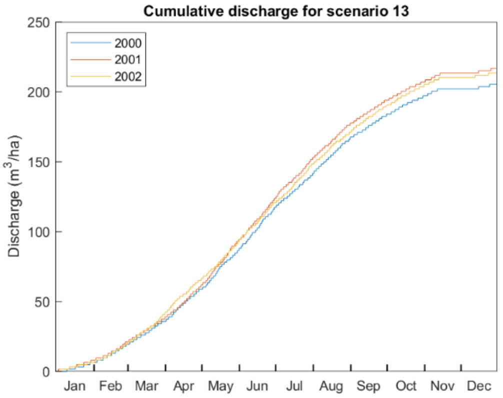

Sodium concentration in scenario 10
Na concentration (mmol/l)
9
8
7
6
5
4
3
2
1
0
2000
2001
2002
2003

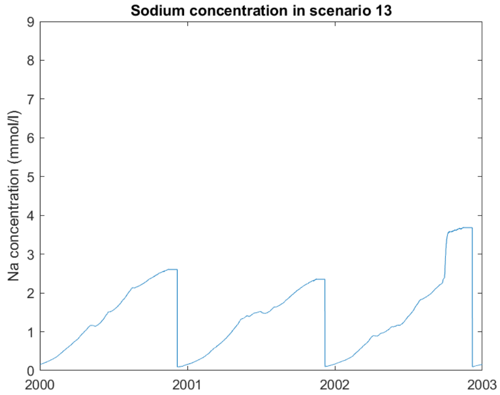

Cumulative discharge for scenario 11
Discharge (m³/ha)
150
100
50
0
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

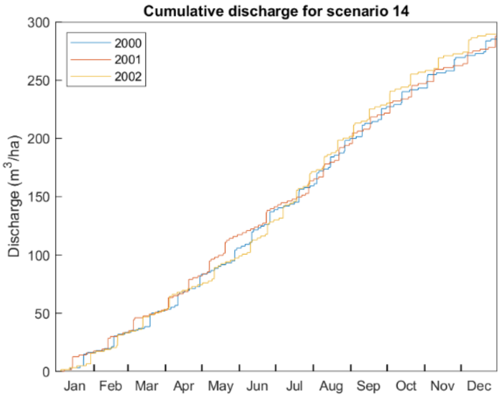

Sodium concentration in scenario 11
Na concentration (mmol/l)
9
8
7
6
5
4
3
2
1
0
2000
2001
2002
2003

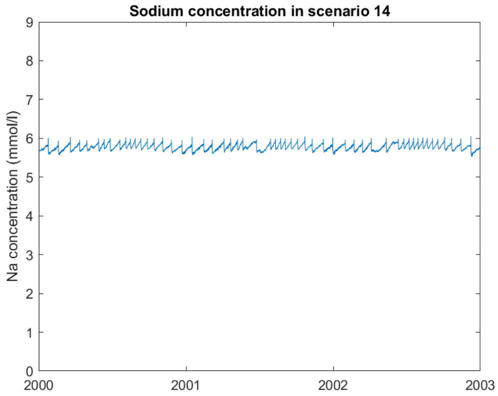

Cumulative discharge for scenario 12
Discharge (m³/ha)
500
450
400
350
300
250
200
150
100
50
0
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

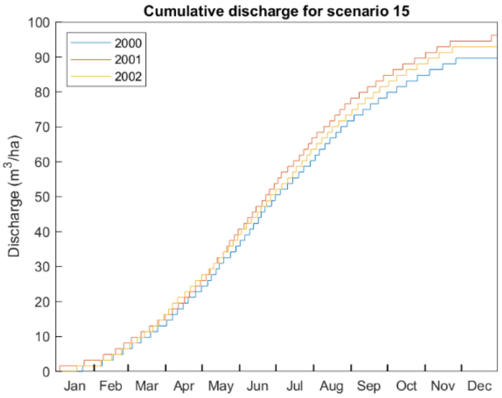

Sodium concentration in scenario 12
Na concentration (mmol/l)
9
8
7
6
5
4
3
2
1
0
2000
2001
2002
2003

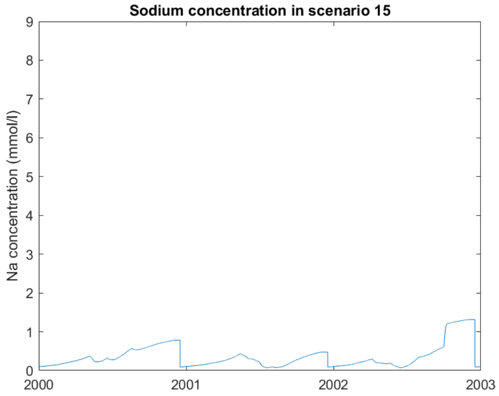

Cumulative discharge for scenario 13

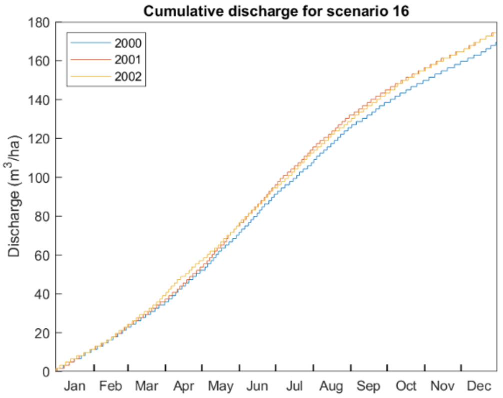

Sodium concentration in scenario 13

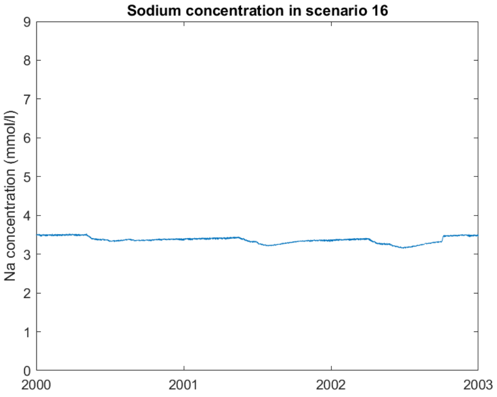

Cumulative discharge for scenario 14

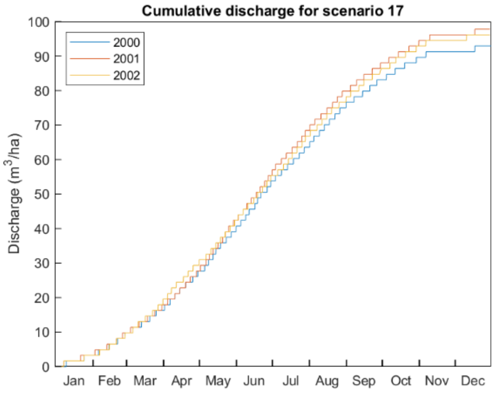

Sodium concentration in scenario 14

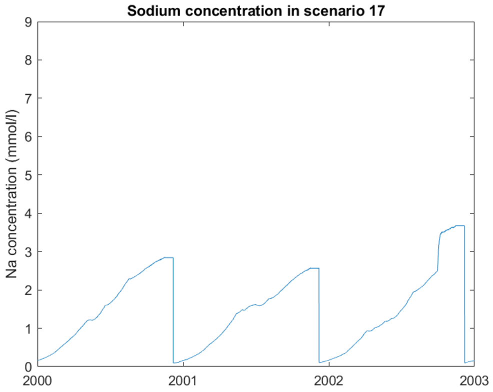

Cumulative discharge for scenario 15

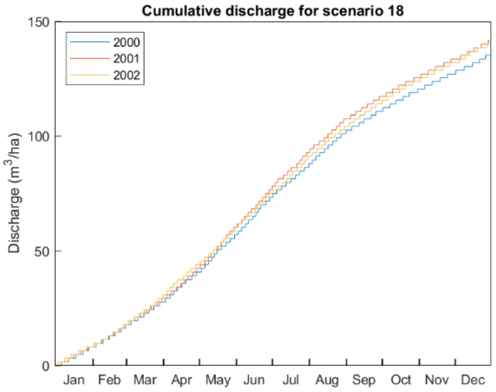

Sodium concentration in scenario 15

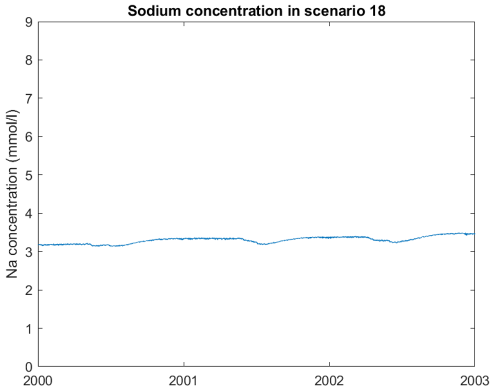

Cumulative discharge for scenario 16

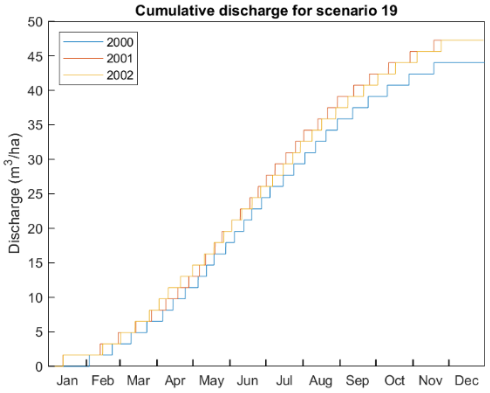

Sodium concentration in scenario 16

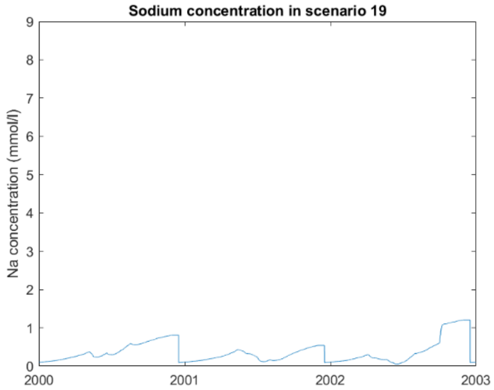

Cumulative discharge for scenario 17
Discharge (m^3/ha)
0
10
20
30
40
50
60
70
80
90
100
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

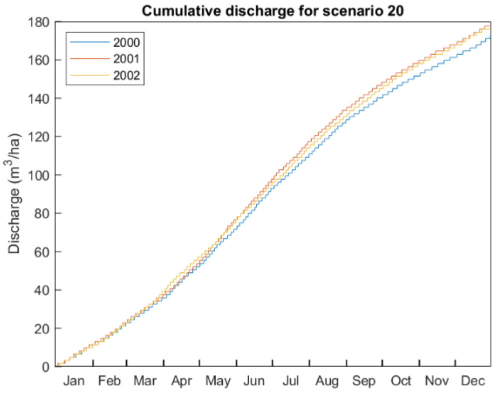

Sodium concentration in scenario 17
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

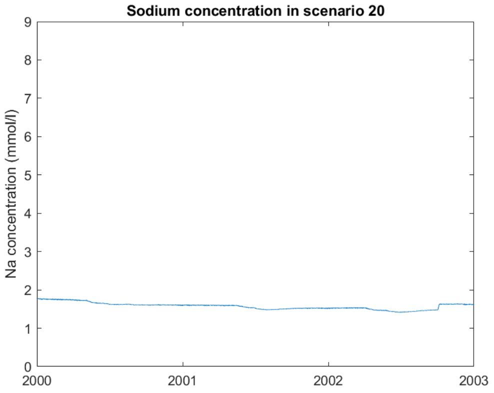

Cumulative discharge for scenario 18
Discharge (m^3/ha)
0
50
100
150
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

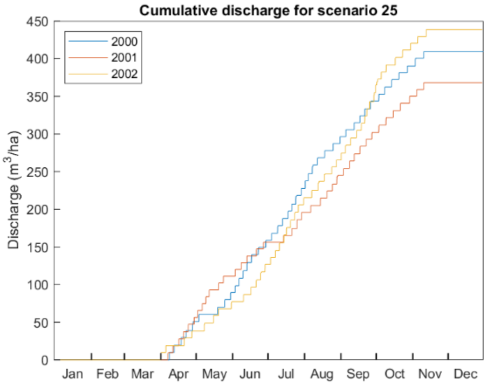

Sodium concentration in scenario 18
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

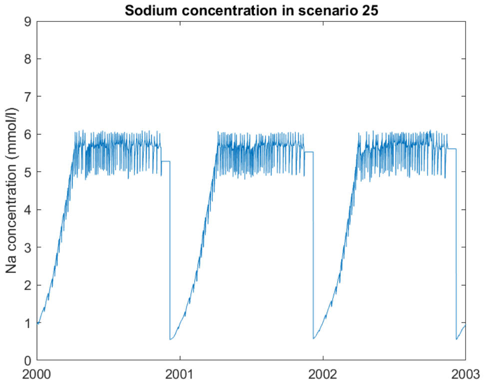

Cumulative discharge for scenario 19
Discharge (m^3/ha)
0
5
10
15
20
25
30
35
40
45
50
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

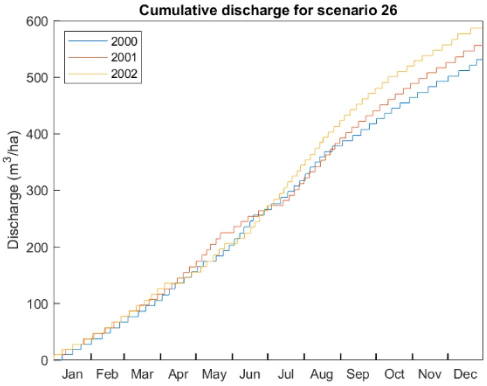

Sodium concentration in scenario 19
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

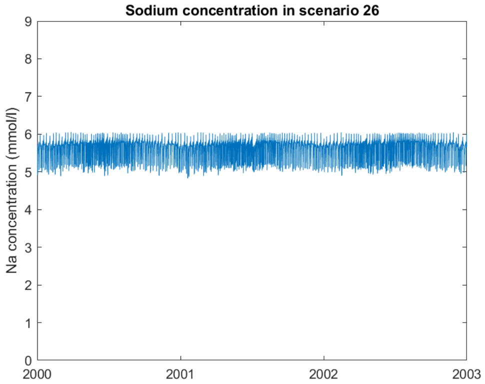

Cumulative discharge for scenario 20
Discharge (m^3/ha)
0
20
40
60
80
100
120
140
160
180
2000
2001
2002
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

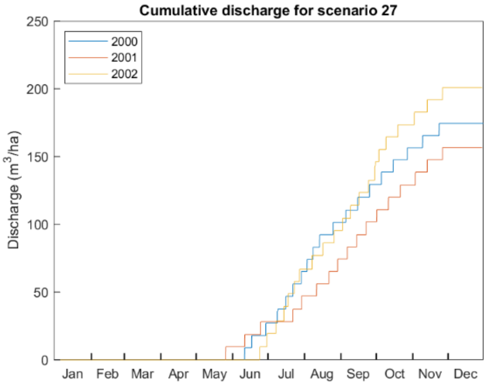

Sodium concentration in scenario 20
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

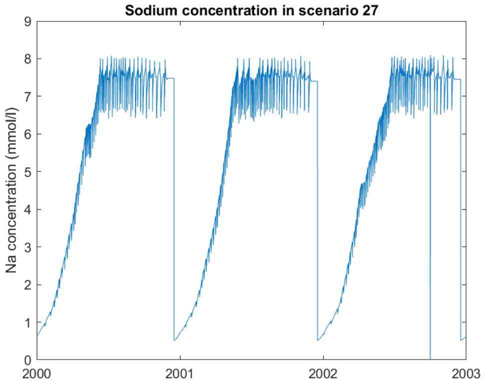

Cumulative discharge for scenario 25
2000
2001
2002
Discharge (m^3/ha)
0
50
100
150
200
250
300
350
400
450
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

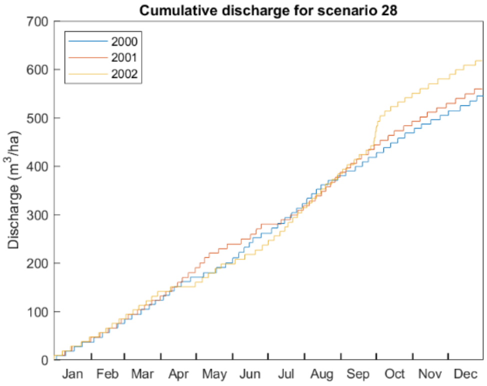

Sodium concentration in scenario 25
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

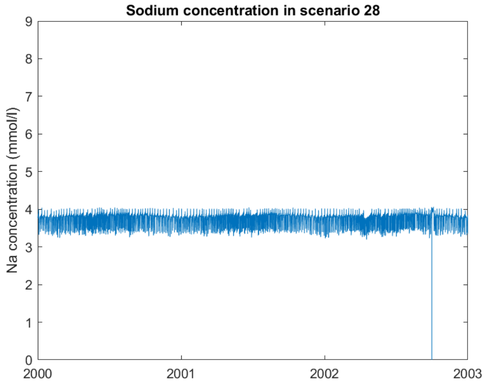

Cumulative discharge for scenario 26
2000
2001
2002
Discharge (m^3/ha)
0
100
200
300
400
500
600
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

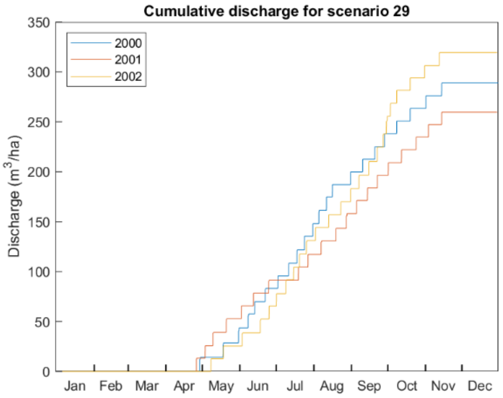

Sodium concentration in scenario 26
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

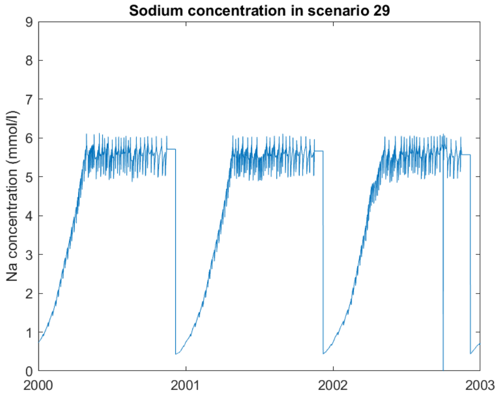

Cumulative discharge for scenario 27
2000
2001
2002
Discharge (m^3/ha)
0
50
100
150
200
250
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

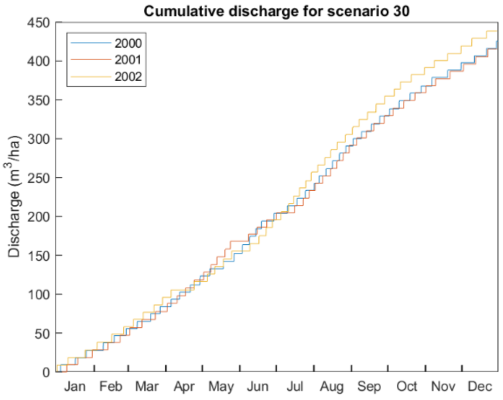

Sodium concentration in scenario 27
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

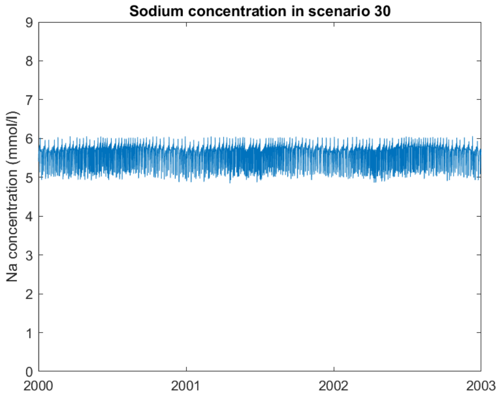

Cumulative discharge for scenario 28
2000
2001
2002
Discharge (m^3/ha)
0
100
200
300
400
500
600
700
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

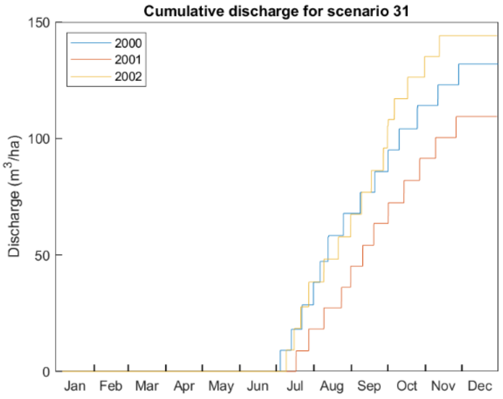

Sodium concentration in scenario 28
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

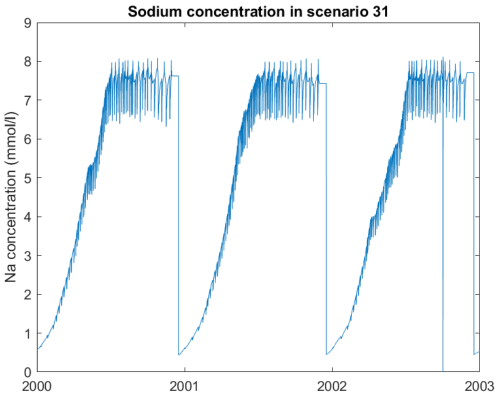

Cumulative discharge for scenario 29
Discharge (m^3/ha)
0
50
100
150
200
250
300
350
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

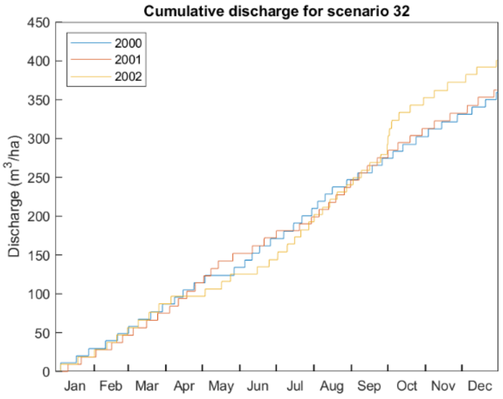

Sodium concentration in scenario 29
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

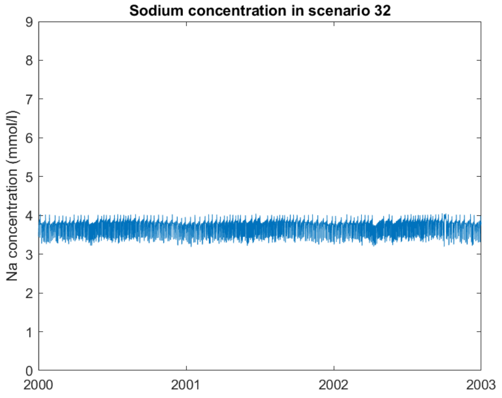

Cumulative discharge for scenario 30
Discharge (m^3/ha)
0
50
100
150
200
250
300
350
400
450
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

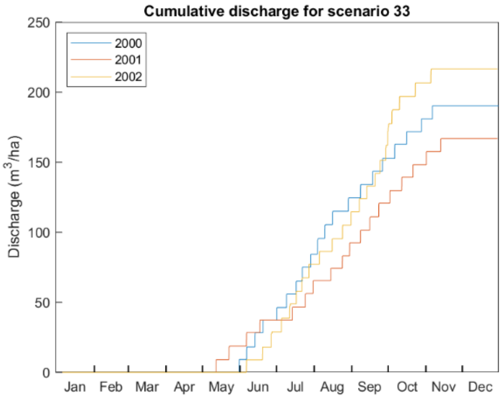

Sodium concentration in scenario 30
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

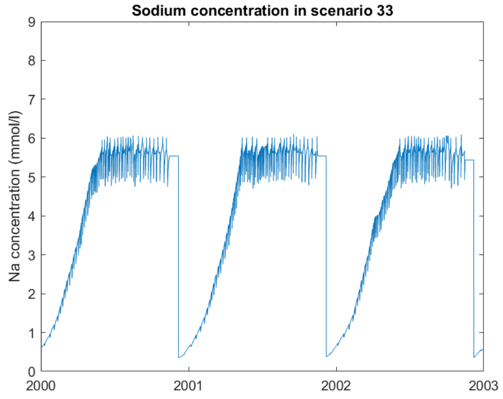

Cumulative discharge for scenario 31
Discharge (m^3/ha)
0
50
100
150
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

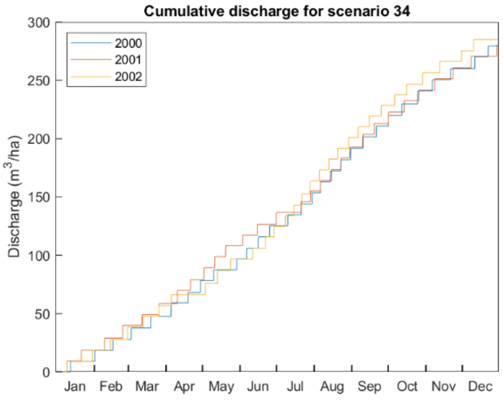

Sodium concentration in scenario 31
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

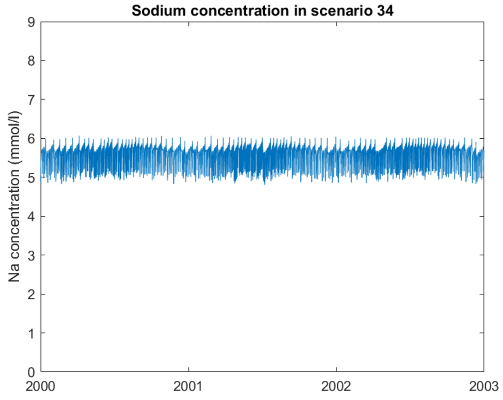

Cumulative discharge for scenario 32
Discharge (m^3/ha)
0
50
100
150
200
250
300
350
400
450
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

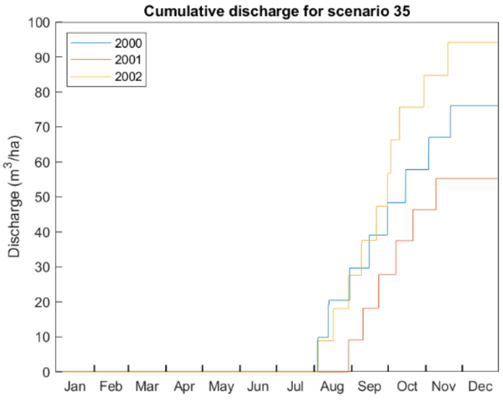

Sodium concentration in scenario 32
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

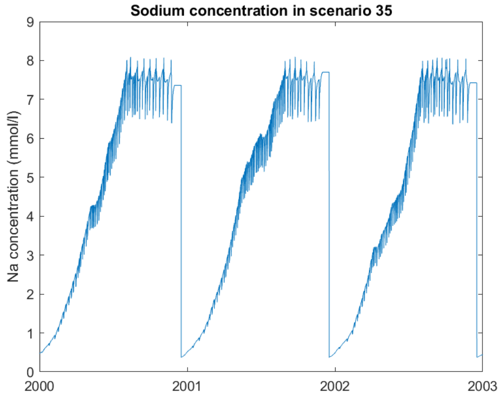

Cumulative discharge for scenario 33

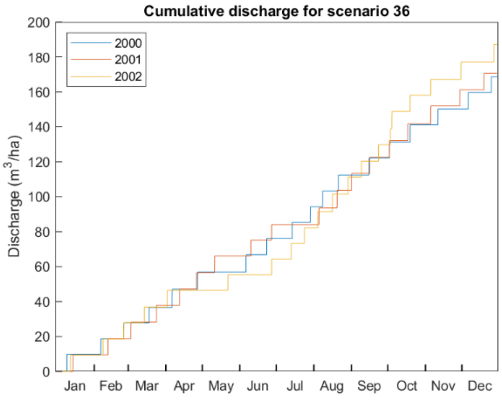

Sodium concentration in scenario 33

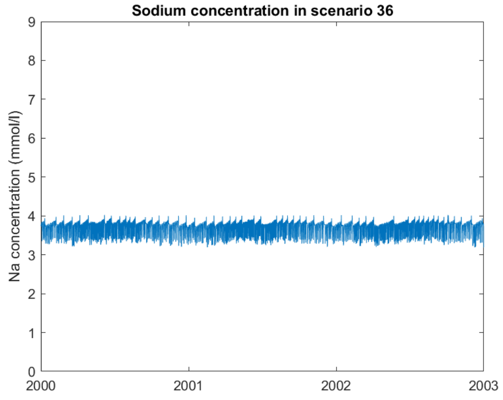

Cumulative discharge for scenario 34

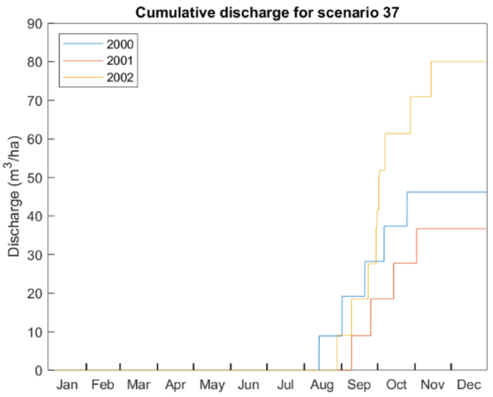

Sodium concentration in scenario 34

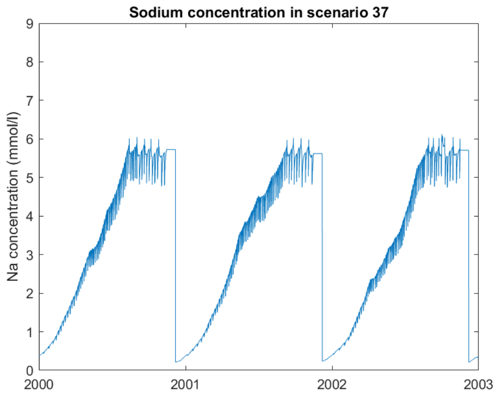

Cumulative discharge for scenario 35

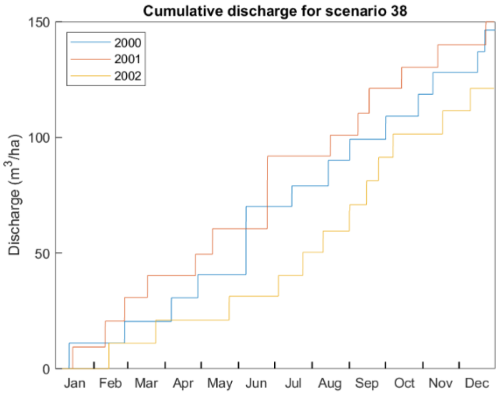

Sodium concentration in scenario 35

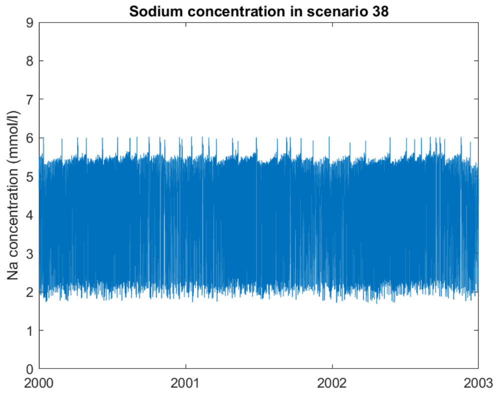

Cumulative discharge for scenario 36

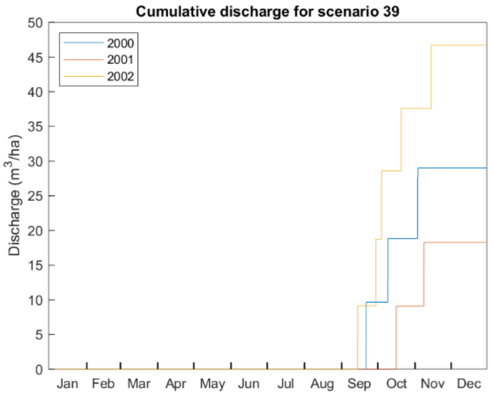

Sodium concentration in scenario 36

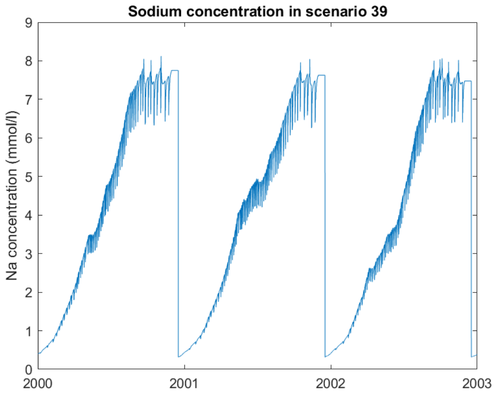

Cumulative discharge for scenario 37
Discharge (m^3/ha)
0
10
20
30
40
50
60
70
80
90
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec

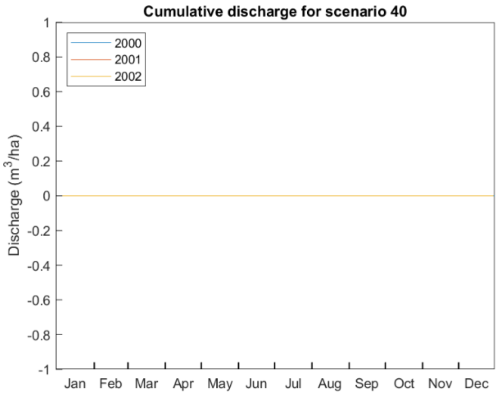

Sodium concentration in scenario 37
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

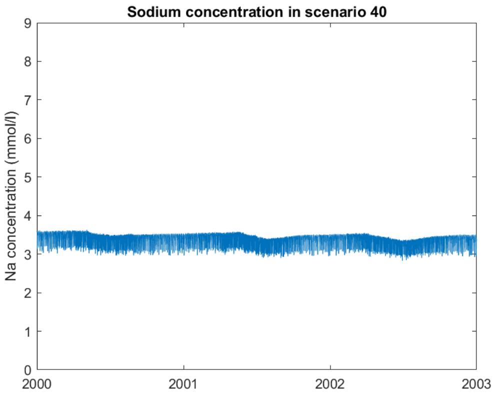

Cumulative discharge for scenario 38
Discharge (m^3/ha)
0
50
100
150
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec


Sodium concentration in scenario 38
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003


Cumulative discharge for scenario 39
Discharge (m^3/ha)
0
5
10
15
20
25
30
35
40
45
50
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec


Sodium concentration in scenario 39
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003


Cumulative discharge for scenario 40
Discharge (m^3/ha)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
2000
2001
2002
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec


Sodium concentration in scenario 40
Na concentration (mmol/l)
0
1
2
3
4
5
6
7
8
9
2000
2001
2002
2003

Annex 5 Deposition on crops in soilless cultivation

Source
In the GEM model the initial deposition on the crop, directly after application is one of the model settings that needs to be defined. Data on this deposition as percentage of the total application is scarce. Ludeking (see Source 1 below) collected data by *WUR Greenhouse Horticulture* for crops grown in Dutch greenhouses, for direct spraying and for Low Volume Misting. Also in the FOCUS groundwater scenarios document tables can be found on the percentage of application which is deposited on the crop (see Source 2 below). These percentages are specific for field crops and for spray application.

Sensitivity of the model
A sensitivity analyses of the model showed that the GEM model (with the implemented concepts as described in this report is sensitive to the percentage of substance applied to the crop.

The model sensitivity was assessed for SEM-S with spray application. In the sensitivity analysis it was assumed that the deposition on the roof, the mats and the troughs is fixed, to 0.1%, 1% and 0.3%. Only the division between the crop and the floor was varied. The sensitivity analysis showed that the model is not sensitive to these changes for most of the substances, except for substances with a high solubility and a high vapour pressure the model is sensitive. When the deposition on the crop is divided by two, the maximum concentration in the drainage tank is 15 to 30% higher, dependent on the season (summer or winter). For assessing the risk of pesticide use the deposition on the crop is therefore better underestimated than overestimated.

We hypothesise that the model will react similarly for LVM application. For LVM, part of the pesticide will initially enter the greenhouse air (to saturated vapour pressure), but the other parameters will be more or less similar. For SEM-P the model will probably be more sensitive to the percentage of the substance applied to the crop, the less is applied the more will be applied to the tables. Via the ebb and flood system the applied mass to the tables becomes directly part of the recirculation water. Also for these systems by underestimating the mass applied to the crops the model will probably overestimate the concentration in the recirculation water.

Registration context
Currently the GEM model does not distinguish between BBCH stages of crops. The rationale behind this approach is that most greenhouse crops arrive quickly to a mature stage. Product registration is generally for crop stage 10-90, hence it includes the leave development stage. The DTG list of the crops that are grown, which is taken up in the model, does not consider small plants, except for garden cress and other vegetable sprouts.

Proposal for GEM 4.4
Given the limited data available of which part is from field crops, SEM-B will not distinguish between types of crops, BBCH crop stages or types of applications (LVM, spray). The depositions on the roof, the troughs, the mats and the greenhouse air will be taken as proposed by Boesten et al. (2019). For the division between the floor and the crops one value will be used which is on the 'safe' side, i.e. it will underestimate the deposition on the crop rather than on the floor/ tables and is valid for BBCH stages 10-90.

Given the data we have, the proposed division is 40% on the crops and 60% on the floor/tables.

Sources of information

Source 1: GEM3.3.2
In GEM 3.3.2 the division of pesticide over the floor, the air and the plant depends on the application type (spraying or LVM/fogging) and on the plant type.

Table 8 *Distribution of a pesticide application by spraying over the different substance compartments in the greenhouse in SEM-S for the reference deposition crops (see Table B-2 of van der Linden et al., 2015).*

Crop type (reference deposition crops)	Fraction of applied dose		
	Deposited on crop surface	Deposited on floor	Staying in greenhouse air
Cut flowers	0.80	0.12	0.08
Lettuce	0.80	0.12	0.08
Tomato and cucumber	0.72	0.20	0.08
Rose and gerbera	0.80	0.12	0.08
Very small young plants	0.00	0.92	0.08

Table 9 *Distribution of a pesticide application by the low volume mister over the different substance compartments in the greenhouse in GEM-B.*

Crop type (reference deposition crops)	Fraction of applied dose		
	deposited on crop surface	deposited on floor	staying in greenhouse air
Cut flowers	0.55	0.10	0.35
Lettuce	0.55	0.10	0.35
Tomato and cucumber	0.55	0.10	0.35
Rose and gerbera	0.55	0.10	0.35
Very small young plants	0	0.65	0.35

These fractions are based on the excel overview developed by D. Ludeking in 2011 (see table next page).

Werkdocument 30-nov-11

Toedieningsmethoden van gewasbeschermingsmiddelen

Toedieningsmethode	**gewas**	**dosering gewasbeschermings-middel**	**watervolume**	**watervolume**	**druppelgrootte**	**percentage depositie gewas/depositie niet-gewas**			
			in liters/ha	in liters/ha	in µ	gewas	substraat/	kasdek	lucht
			jong gewas	volgroeid gewas			bodem		(afh. Vp van middel
						(volgroeid	(volgroeid		en dichtheid gewas)
						gewas)	gewas)		39 % bij Vp>10
									bij Vp 0,01 - 10
gewasbehandelingen									
hoog-volume		ml of g / 100 l							
	snijbloemen, potplanten,		400	1000	10 - 400	70-90	5 - 15	< 1	8 - 10
	sla, radijs		400	600	10 - 400	70-90	5 - 15	< 1	8 - 10
	tomaat, komkommer		400	1500	10 - 400	70-90	15-30	< 1	8 - 10
	roos, gerbera		400	2500	10 - 400	70-90	5 - 15	< 1	8 - 10
	opkweek***		400	600	10 - 400				8 - 10
ruimtebehandelingen									
laag-volume: LVM		hoeveelheid middel voor 1000 liter water in 10 liter							
	snijbloemen, potplanten,		10	10	10 - 30	50-60	5 - 10	1-5	20-25
	sla, radijs		10	10	10 - 30	50-60	5 - 10	1-5	20-25
	tomaat, komkommer		10	10	10 - 30	50-60	5 - 10	1-5	20-25
	roos, gerbera		10	10	10 - 30	50-60	5 - 10	1-5	20-25
	opkweek***		10	10	10 - 30				20-25
laag-volume: foggen (gasnevelen)		hoeveelheid middel voor 1000 liter water in 10 liter							
	snijbloemen, potplanten,		10	10	5 (<10)	50-60	5 - 10	1-5	20-25
	sla, radijs		10	10	5 (<10)	50-60	5 - 10	1-5	20-25
	tomaat, komkommer		10	10	5 (<10)	50-60	5 - 10	1-5	20-25
	roos, gerbera		10	10	5 (<10)	50-60	5 - 10	1-5	20-25
substraatbehandeling									
aangieten/druppelen		volgens etiket							
	potplanten,	100 ml / plant*						< 1**	< 1**
	tomaat, komkommer	100 ml / plant*						< 1**	< 1**
	roos, gerbera	100 ml / plant*						< 1**	< 1**
	sla, radijs	l of g /100 m2						< 1**	< 1**
	opkweek***	l of g /100 m2							

* middel + water

** geen metingen

*** opkweek vruchtgroenten , lijkt sterk op potplanten

gasnevelen - cijfers zijn gebaseerd op LVM

Alle cijfers zijn gemiddelden

Eb/vloed - geen cijfers gevonden

Source 2: FOCUS groundwater
Values for arable crops and trees can be found on the CTGB website: https://english.ctgb.nl/plant-protection/documents/assessment-framework-ppp/2019/03/01/content-6.-environmental-fate--behaviour-em2019-2 (source: FOCUS groundwater interception tables Annex 3 (interception values per crop stage) and 4 (linking to DTG crops)).

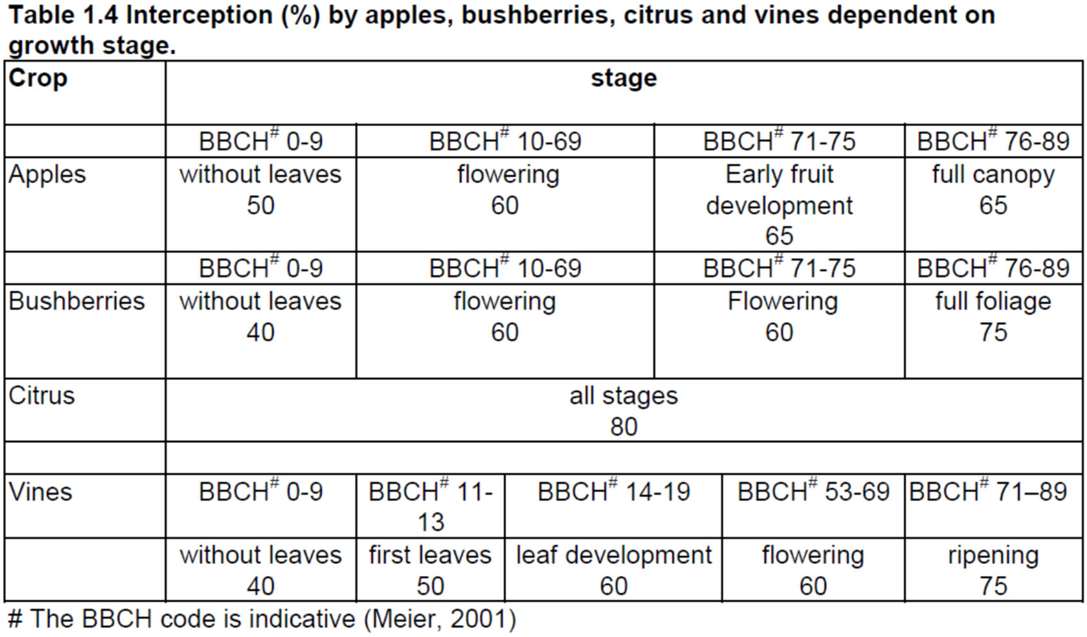


Table 1.4 Interception (%) by apples, bushberries, citrus and vines dependent on growth stage.

<table>
<tr><th>Crop</th><th colspan="6">stage</th></tr>
<tr><td></td><td>BBCH# 0-9</td><td colspan="2">BBCH# 10-69</td><td colspan="2">BBCH# 71-75</td><td>BBCH# 76-89</td></tr>
<tr><td>Apples</td><td>without leaves
50</td><td colspan="2">flowering
60</td><td colspan="2">Early fruit development
65</td><td>full canopy
65</td></tr>
<tr><td></td><td>BBCH# 0-9</td><td colspan="2">BBCH# 10-69</td><td colspan="2">BBCH# 71-75</td><td>BBCH# 76-89</td></tr>
<tr><td>Bushberries</td><td>without leaves
40</td><td colspan="2">flowering
60</td><td colspan="2">Flowering
60</td><td>full foliage
75</td></tr>
<tr><td>Citrus</td><td colspan="6">all stages
80</td></tr>
<tr><td></td><td colspan="6"></td></tr>
<tr><td>Vines</td><td>BBCH# 0-9</td><td>BBCH# 11-13</td><td colspan="2">BBCH# 14-19</td><td>BBCH# 53-69</td><td>BBCH# 71–89</td></tr>
<tr><td></td><td>without leaves
40</td><td>first leaves
50</td><td colspan="2">leaf development
60</td><td>flowering
60</td><td>ripening
75</td></tr>
</table>

The BBCH code is indicative (Meier, 2001)

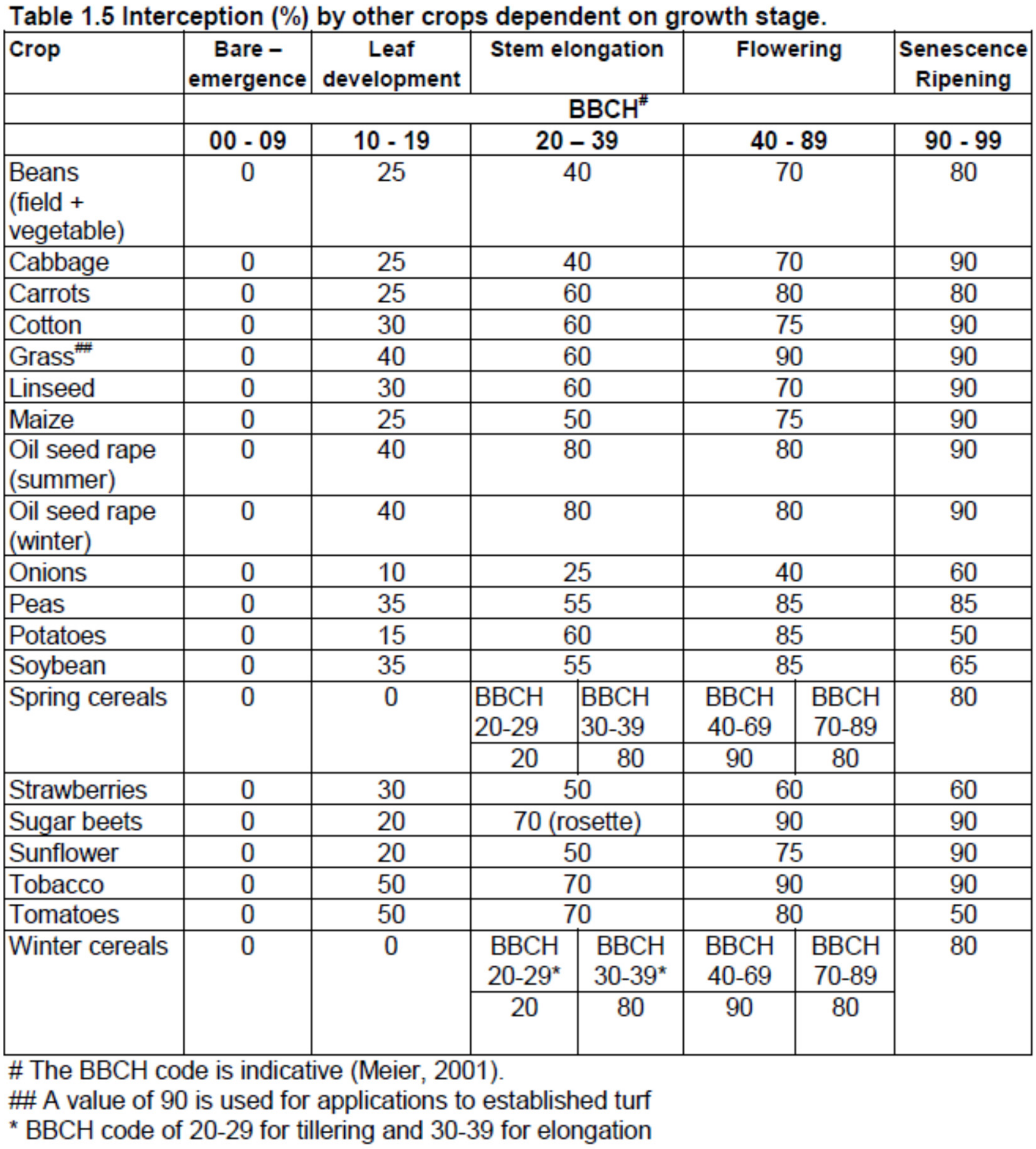


Table 1.5 Interception (%) by other crops dependent on growth stage.

Crop	Bare – emergence	Leaf development	Stem elongation		Flowering		Senescence Ripening
	BBCH#						
	00 - 09	10 - 19	20 – 39		40 - 89		90 - 99
Beans (field + vegetable)	0	25	40		70		80
Cabbage	0	25	40		70		90
Carrots	0	25	60		80		80
Cotton	0	30	60		75		90
Grass##	0	40	60		90		90
Linseed	0	30	60		70		90
Maize	0	25	50		75		90
Oil seed rape (summer)	0	40	80		80		90
Oil seed rape (winter)	0	40	80		80		90
Onions	0	10	25		40		60
Peas	0	35	55		85		85
Potatoes	0	15	60		85		50
Soybean	0	35	55		85		65
Spring cereals	0	0	BBCH 20-29	BBCH 30-39	BBCH 40-69	BBCH 70-89	80
			20	80	90	80	
Strawberries	0	30	50		60		60
Sugar beets	0	20	70 (rosette)		90		90
Sunflower	0	20	50		75		90
Tobacco	0	50	70		90		90
Tomatoes	0	50	70		80		50
Winter cereals	0	0	BBCH 20-29*	BBCH 30-39*	BBCH 40-69	BBCH 70-89	80
			20	80	90	80	

The BBCH code is indicative (Meier, 2001).
A value of 90 is used for applications to established turf
* BBCH code of 20-29 for tillering and 30-39 for elongation

Source 3: Suggestions by Boesten et al. (2019) for new GEM
In Boesten et al. (2019) Table 10 Table 11 were suggested. The new concepts of GEM have no initial pesticide concentration in the greenhouse air for spray application and a concentration at saturated vapour pressure for LVM applications. Also deposition om mats, troughs, and roof are considered.

The deposition on crop and floor is calculated back from Table 8 and Table 9. E.g. for cut flowers the deposition on the crop was originally 0.80, this was based on 8% of the applied mass in the greenhouse air. In the new model 1.4% is applied on roof, mats or troughs. Hence, 0.80/0.92*0.986 = 0.857 etc.

Table 10 *Recommended initial distribution of pesticide after spray applications for the reference deposition crops.*

Reference deposition crop	**Fraction of applied dose**				
	Deposited on crop surface	**Deposited on floor**	**Deposited on roof**	**Dripped into mats**	**Deposited on troughs**
Cut flowers	0.857	0.129	0.001	0.01	0.003
Lettuce	0.857	0.129	0.001	0.01	0.003
Tomato and cucumber	0.772	0.214	0.001	0.01	0.003
Rose and gerbera	0.857	0.129	0.001	0.01	0.003
Very small young plants	0.00	0.989	0.001	0.01	0.003

Table 11 *Recommended initial distribution of pesticide after LVM applications for the reference deposition crops. These fractions apply to the applied mass per surface area of greenhouse (A_i) minus the mass per surface area of greenhouse corresponding with the saturated vapour concentration ($A_{a,sat}$) because it is assumed that the concentration in the air initially is equal to this concentration.*

Reference deposition crop	**Fraction of (A_i - $A_{a,sat}$)**				
	Deposited on crop surface	**Deposited on floor**	**Deposited on roof**	**Dripped into mats**	**Deposited on troughs**
Cut flowers	0.827	0.150	0.010	0.010	0.003
Lettuce	0.827	0.150	0.010	0.010	0.003
Tomato and cucumber	0.827	0.150	0.010	0.010	0.003
Rose and gerbera	0.827	0.150	0.010	0.010	0.003
Very small young plants	0.000	0.977	0.010	0.010	0.003

Annex 6 Procedure to update masses in GEM

The explicit scheme to solve the differential equations describing the reservoirs outside of the recirculation water may result in a negative mass when mass for the previous time step is close to zero and relatively strong loss fluxes occur (see also Figure 13). Correction by simply setting negative masses to zero is not sufficient. Additionally loss fluxes should adjusted downward, otherwise mass balance errors would occur when the loss fluxes flow to a different reservoirs (mass would be created). However, these masses of the receiving reservoirs then need to be recalculated as well, based on the adjusted flux.

To solve this problem we implemented a iterative procedure to calculate the fluxes and update the masses. We demonstrate this procedure based on a hypothetical system with two connected reservoirs depicted in Figure 12. Loss fluxes are assumed to be a function of the donor reservoir and hence the correction is made in the incoming fluxes.

With the standard explicit scheme the masses at timestep $\mathrm{t}+1$ are calculated as follows:

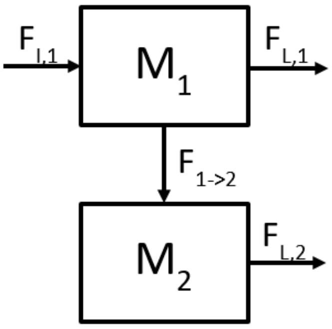


Figure 12 *System with two connected reservoirs.*

$$M_1^{t+1} = M_1^t + \Delta t\ \left(F_{I,1} - F_{1\to2}(M_1^t) - F_{L,1}(M_1^t)\right)$$
$$M_2^{t+1} = M_2^t + \Delta t\ \left(F_{1\to2}(M_1^t) - F_{L,2}(M_2^t)\right)$$

where*:*
M_j^t: mass in reservoir *j* at time step *t*
Δt: time step length
$F_{I,1}$: input mass flux into reservoir 1
$F_{1\to2}(M_1^t)$: mass flux from reservoir 1 to reservoir 2 as a function of M_1^t
$F_{L,j}\left(M_j^t\right)$: loss mass flux from reservoir *j* (function of M_j^t; leaves system)

Iteration procedure

For the purpose of iteration we introduce the following variables:

i: iteration step

f_1^i: scaling factor to reduce loss fluxes for reservoir 1 in iteration step i

ε: minimum value of masses, e.g. -1x10^{-15}

The masses in time step $t+1$ are calculated as follows:

```
Calculate unscaled fluxes: $F_I$, $F_{1\to 2}(M_1^t)$, $F_{L,1}(M_1^t)$ and $F_{L,2}(M_2^t)$
Set $f_1^1, f_2^1 = 1$
Set $i = 1$
Loop until done:
    Calculate "hypothetical" masses for this iteration step:
    $M_1^{i,t+1} = M_1^t + \Delta t \left(F_{I,1} - f_1^i \left( F_{1\to 2}(M_1^t) + F_{L,1}(M_1^t)\right)\right)$
    $M_2^{i,t+1} = M_2^t + \Delta t \left(f_1^i F_{1\to 2}(M_1^t) - f_2^i F_{L,2}(M_2^t)\right)$
    If $\left(M_1^{i,t+1} > \varepsilon \text{ and } M_2^{i,t+1} > \varepsilon\right)$ then
        Set masses for next time step:
        $M_1^{t+1} = M_1^{i,t+1}$
        $M_2^{t+1} = M_2^{i,t+1}$
        Exit loop
    Else
        If $\left(M_1^{i,t+1} < \varepsilon\right)$ then
            Recalculate scaling factor to reduce loss fluxes:
            $f_1^{i+1} = \frac{\frac{f_1^i( F_{1\to 2} + F_{L,1}) + M_1^{i,t+1}}{\Delta t}}{f_1^i( F_{1\to 2} + F_{L,1})}$
        End if
        If $\left(M_2^{i,t+1} < \varepsilon\right)$ then
            Recalculate scaling factor to reduce loss fluxes:
            $f_2^{i+1} = \frac{f_2^i F_{L,2}(M_2^t) + M_2^{i,t+1}/\Delta t}{f_2^i F_{L,2}(M_2^t)}$
        End if
        Set: $i = i + 1$
    End if
End loop
```

This procedure is applied to update all compartments outside the recirculation water in SEM-S and SEM-P (Figure 13).

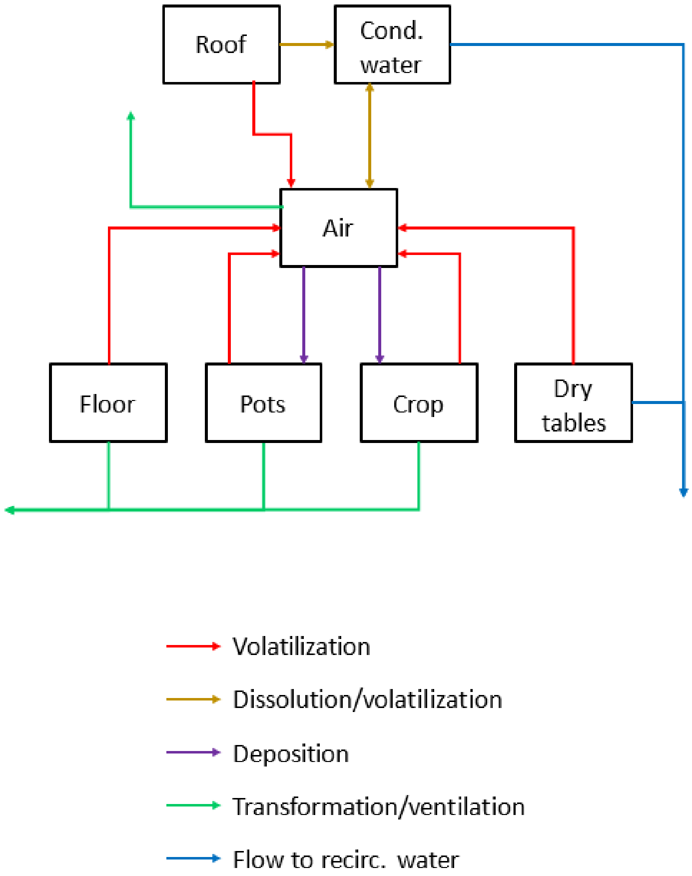


Figure 13 *Reservoirs outside the recirculation water to which the described procedure is applied.*

Annex 7 Parameter values used in SEM-S and SEM-P

Table 12 *Parameter values.*

Name in code	Description	Unit	Value	Source of value
masFoi	Mass of foil per ha greenhouse, corrected for contact with water	kg/ha	50.835	See Table A6.2
masSubSor	Mass of wet substrate, contributing to sorption	kg/ha	13300	See Table A6.2
masWetRts	Mass of wet roots	kg/ha	9500	See Table A6.2
LenPolIrrTub	Length of polyethylene irrigation tubes	m/ha	6240	See Table A6.2
InnSurArePolIrrTub	Surface area of cross section of polyethylene irrigation tubes	m^2	3.80E-04	See Table A6.2
MasPerLenPolIrrTub	Mass per length of polyethylene irrigation tubes	kg/m	0.5	See Table A6.2
LenPolCapTub	Length of polyethylene capillary tubes	m/ha	20000	See Table A6.2
InnSurArePolCapTub	Surface area of cross section of polyethylene capillary tubes	m^2	7.07E-06	See Table A6.2
MasPerLenPolCapTub	Mass per length of polyethylene capillary tubes	kg/m	0.015	See Table A6.2
LenPvcTub	Length of PVC transport tubes	m/ha	832	See Table A6.2
InnSurArePvcTub	Surface area of cross section of PVC transport tubes	m^2	8.17E-03	See Table A6.2
MasPerLenPvcTub	Mass per length of PVC transport tubes	kg/m	1.57	See Table A6.2
NumComPot	Number of layers for numerical solution of transport in pots	-	50	This report
GAI	Glass area index, area of roof glass per area greenhouse	-	1.18	Kempkes et al., 2018
FacVolRoo	Proportionality factor for calculating volatisation of substance from roof	-	0.01	Boesten et al., 2019
FacDslCnd	Proportionality factor for calculating dissolution of substance into condensation water	-	0.07	Boesten et al., 2019
FacVolCrp	Factor describing deviation of concentration in air above plant surface from saturated concentration	-	0.2	Boesten et al., 2019
FraDepFlr	Fraction of floor surface contaminated with deposits during application	-	0.5	van Os, pers. comm.
RstAirLay	Laminar boundary layer resistance	d/m	2.31E-03	Boesten et al., 2019
HghPotUppLay	Thickness of upper layer in pots in which transport occurs	m	0.05	Boesten et al., 2019
FraWatPot	Fraction of water in upper layer of pots (not in contact with table water)	-	0.3	Boesten et al., 2019
IrrWaiTim	Wait time between spray or LVM application and irrigation in SEM-P	d	1	van Os, pers. comm.
RelErrTolCrc	Tolerance for relative mass balance errors in recirculation water	-	1.00E-10	
RelErrTolAbg	Tolerance for relative mass balance errors in aboveground system	-	1.00E-10	
RelErrTolGh	Tolerence for relative mass balance errors in total greenhouse	-	1.00E-10	
MasNegTolAbgLoc	Tolerence for negative mass in above ground compartment	kg/m^2	0.00E+00	

Name in code	Description	Unit	Value	Source of value
FraCulTank1	Fraction of substrate in first substrate layer	-	0.5	This report
FraPvcTub1	Fraction of PVC transport tubes in first substrate layer	-	0.5	This report
FraPolCapTub1	Fraction of polyethylene capillary tubes in first substrate layer	-	1	This report
FraWetRts1	Fraction of wet roots in first substrate layer	-	1	This report
PhiPts	Porosity of soil in pots	-	0.6	Van der Linden et al., 2015
RhoPts	Bulk density of soil in pots	kg m^{-3}	1000	Van der Linden et al., 2015
CntOmPts	Organic matter content of soil in pots	-	0.1	Van der Linden et al., 2015
FacUptMax	Parameter of function describing relationship between K_{ow} and root uptake: maximum uptake factor.	-	0.784	Briggs et al., 1982
FacUptMaxMaxLoc	Parameter of function describing relationship between K_{ow} and root uptake: log-K_{ow} value where uptake factor is maximal.	-	1.78	Briggs et al., 1982
FacUptShp	Parameter of function describing relationship between K_{ow} and root uptake: shape parameter	-	2.44	Briggs et al., 1982
AvoGHAir	Areic volume of greenhouse air (average height of greenhouse ceiling)	m^3 m^{-2}	6	Van der Linden et al., 2015
NVent	Ventilation rate	d^{-1}	50	Van der Linden et al., 2015
Agh	Surface area of the greenhouse	m^2	10000	
AvoCnd	Areic volume of condensation water	m^3 m^{-2}	0.000532	Van der Linden et al., 2015
TankMaxSize(1)	Maximum size of used-water tank	m^3	35	Wipfler et al., 2020
TankMaxSize(2)	Maximum size of clean-water tank	m^3	70	Wipfler et al., 2020
TankMinSize(1)	Minimum size of used-water tank	m^3	1.5	
TankMinSize(2)	Minimum size of clean-water tank	m^3	0	
TankSize(3)	Fixed size of wastewater tank	m^3	2	
TankSize(4)	Fixed size of mixing tank	m^3	50	Wipfler et al., 2020
TankSize(5)	Fixed size of cultivation tank	m^3	95	Wipfler et al., 2020
TankSize(6)	Fixed size of drainwater tank	m^3	2	
TankSize(7)	Fixed size of filter tank	m^3	0.125	
TankSize(8)	Fixed size of disinfection tank	m^3	0.125	
-	Temperature difference between greenhouse air and ‘cold’ tanks: mixing, used water, filter, disinfection, clean water	ºC	2	

Table 13 *Parameters used to calculate properties of stonewool substrate, foil and roots*

Variable	Units	Value	Source
Input			
Height substrate slab	cm	7.5	van Os (pers. comm.)
Width substrate slab	cm	15	van Os (pers. comm.)
Length substrate slab	cm	100	van Os (pers. comm.)
Two sided surface area of foil per mass of foil	cm^2/g	281	Boesten & Matser, 2017 (p. 12)
Water content slab	-	0.7	van Os (pers. comm.)
Correction factor for slab circumference vs foil area per cm slab length	-	1.015789474	Boesten & Matser, 2017 (p. 12)
Number of slabs per ha greenhouse	#/ha	12500	van Os (pers. comm.)
Correction factor for the fact that only inside part of foil is in contact with water	-	0.5	Boesten et al., 2019 (p. 16)
Correction factor to account for incomplete contact between foil and water in substrate	-	0.5	Boesten et al., 2019 (p. 16)
Mass of substrate per unit volume of water in cultivation tank	g/cm^3	0.14	Boesten et al., 2019 (p. 17)
Mass of wet roots per unit volume of water in cultivation tank	kg/dm^3	0.1	Boesten et al., 2019 (p. 20)
Total volume of water in cultivation tank in SEM	m^3/ha	95	
Substrate slabs, volume			
Total length of slab per ha greenhouse	cm	1250000	
Total slab volume per cm length	cm^3/cm	112.5	
Total volume slab per ha greenhouse	cm^3/ha	140625000	
Total volume slab per ha greenhouse	m^3/ha	140.625	
Volume of water in slabs per cm length	cm^3/cm	78.75	
Substrate slabs, mass			
Mass substrate slab per ha greenhouse	g/ha	13300000	
Mass substrate slab per ha greenhouse	kg/ha	13300	
Roots			
Mass of wet roots per ha greenhouse	kg/ha	9500	Based on 95 m3 in cultivation tank
Foil			
Foil area per unit length slab	cm^2/cm	45.71052632	
Foil area per unit bulk volume slab	cm^2/cm^3	0.406315789	
Foil mass per unit length slab	g/cm	0.162670912	
Foil mass per unit bulk volume slab	g/cm^3	0.001445964	
Mass foil per ha greenhouse	g/ha	203338.6402	
Mass of foil per ha greenhouse, corrected for contact with water	g/ha	50834.66005	
Mass of foil per ha greenhouse, corrected for contact with water	kg/ha	50.83466005	

Table 14 *Parameters used to calculate properties of irrigation tubes*

Tube/pipe type	Variable	Value
Polyethylene irrigation tube	length per ha greenhouse (m)	6240
	inner diameter (mm)	22
	mass per length (kg/m)	0.5
	inner surface area (dm^2)	0.038013271
	inner surface area (m^2)	3.80E-04
Polyethylene capillary tube	length per ha greenhouse (m)	20000
	inner diameter (mm)	3
	mass per length (kg/m)	0.015
	inner surface area (dm^2)	0.000706858
	inner surface area (m^2)	7.07E-06
PVC transport tubes	length per ha greenhouse (m)	832
	inner diameter (mm)	102
	mass per length (kg/m)	1.57
	inner surface area (dm^2)	0.817128249
	inner surface area (m^2)	8.17E-03

Table 15 *Crop specific parameters*

Code	Crop name	Reference crop WSM	Reference crop SEM	Mats/Pots	LAI
3.2.4.2	Raspberry	Pepper	Cut flowers & pot plants	Pots	4
4.1.4.1	Witloof Chicory (forced cultivation)	Pepper	Lettuce and radish	Mats	5
4.1.4.2	Watercress	Rose	young plants	Mats	1
4.1.4.4	Rocket	Rose	young plants	Mats	4
4.1.5.1	Garden cress	Rose	young plants	Mats	1
4.1.5.5	Other vegetable sprouts	Rose	young plants	Mats	1
4.3.1.1	Gherkin	Pepper	Tomato and cucumber	Mats	3
4.3.1.2	Zucchini	Tomato	Tomato and cucumber	Mats	6
4.3.1.3	Cucumber	Tomato	Tomato and cucumber	Mats	4
4.3.2.1	Pumpkins	Tomato	Tomato and cucumber	Mats	4
4.3.3.1	Eggplant	Tomato	Tomato and cucumber	Mats	7
4.3.3.2	Tomato	Tomato	Tomato and cucumber	Mats	4
4.3.3.3	Sweet Pepper	Pepper	Tomato and cucumber	Mats	7
5.1.1.1	Basil	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.2	Chives	Plot plant	Cut flowers & pot plants	Pots	2
5.1.1.3	Summer savory	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.4	Lemon balm	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.5	Dill	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.6	Tarragon	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.9	Coriander	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.10	Parsley	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.12	Marjoram	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.13	Oregano	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.14	Mint	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.16	Rosemary	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.17	Sage	Plot plant	Cut flowers & pot plants	Pots	4
5.1.1.18	Thyme	Plot plant	Cut flowers & pot plants	Pots	4
5.3.1.3	Wild pansy	Plot plant	Cut flowers & pot plants	Pots	3
7.1.1.3	Winter Bulb flower and tuber flower for flower/Plot plant cultivation	Rose	Cut flowers & pot plants	Pots	0.5
7.1.1.4	Summer Bulb flower and tuber flower for flower/Plot plant cultivation	Rose	Cut flowers & pot plants	Pots	4
3.2.1	Strawberries	Pepper	Lettuce and radish	Mats	3
4.1.1	Lettuce; Lactuca spp	Pepper	Lettuce and radish	Mats	5

Code	Crop name	Reference crop WSM	Reference crop SEM	Mats/Pots	LAI
7.2.1	Pot plants	Plot plant	Cut flowers & pot plants	Pots	5
7.2.2	Cut flowers	Rose	Rose and gerbera	Mats	5
7.2.3	Forced shrubs	Rose	Cut flowers & pot plants	Pots	5
7.2.4	Cut green	Rose	Cut flowers & pot plants	Pots	6
7.3.2	Climbing plants	Plot plant	Cut flowers & pot plants	Pots	6
7.3.3	Ornamental shrubs (including Roses)	Plot plant	Cut flowers & pot plants	Pots	5
7.3.4	Conifers (including Christmas trees)	Plot plant	Cut flowers & pot plants	Pots	6
7.3.7	Heather	Plot plant	Cut flowers & pot plants	Pots	5
7.4	Perennial crops	Plot plant	Cut flowers & pot plants	Pots	5

Annex 8 Sensitivity of simplified version of SEM-P to presence of permanent water layer on tables for ranges of solubility, saturated vapour pressure and K_{om}

Introduction

The previous version of SEM-P assumed that there was continuously water on the tables. The volume of the water on the tables is 95 m^3/ha, corresponding with a permanent water layer of 0.95 cm (considering the full area of the greenhouse). However, in reality most of the time the tables are dry because irrigation takes place every two or three days and at the start of an irrigation event, a water layer of about 5 cm is formed on the tables which gradually drains away over a period of 15-20 min. Therefore the current version of SEM-P assumes that the tables are dry and that at 1 d after application the remaining amount on the table is dissolved in the irrigation water.

In this annex we assess the probable consequences of this change by calculations with a simplified version of SEM-P considering ranges of solubility, saturated vapour pressure and K_{om}. We expect that the results will be helpful for a more focussed sensitivity analysis of the complete SEM-P model at a later stage.

Calculation procedures

System with dry table at application time

Calculations were made for a simplified version of SEM-P, i.e. a system consisting of plants, pots, roof, greenhouse air, condensation water, and a cultivation tank that contained the irrigation water assuming a constant temperature in the greenhouse of 20°C. Fluxes in the water and gas phase were the same as in the version of GEM described in this report. As in this version, it was assumed that the table is dry for the first day after application during which the amount deposited on the tables may volatilise. After this first day, the remaining amount is taken up by the irrigation water and there is no further volatilisation from or deposition on the irrigation water (because the water is present in a tank). The pesticide present in the condensation water flux was added to the irrigation water and uptake of the pesticide by the pots via the irrigation water was ignored.

Calculations were made for a spray application and parameters as in Table 16 using a volume of the cultivation tank of 125 m^3 with $c_{w,sol}$ ranging between 1 and 1000 mg/L, P_{sat} ranging between 10^{-6} and 3×10^{-3} Pa, and with K_{om} = 0 or 10 000 L/kg. Please note that the final version of GEM 4.4. will use a volume of the cultivation tank of 95 m^3.

The simulation period was limited to 10 days because usually there are emissions to the surface water within 10 days after application. The initial distribution of the dose was as follows: 87% deposited on the plants, 9% on the table, 4% on the pots and 0.1% on the roof (note that these percentages are old values that will be superseded by the revised numbers: 40% deposited on plants, 42% on the table, 18% on the pots and 0.1% on the roof). The output considered was the percentage of the dose present in the cultivation tank assuming that emission loads are approximately proportional to this percentage. So the water in the cultivation tank was considered representative of the recirculation water. Thus the percentage in this water was the sum of two processes: uptake in the irrigation water of the amount remaining on the tables after 1 day and input from the condensation water.

Table 16 *Parameter values as used in the sensitivity analysis of SEM-P.*

Parameter	Value used
b	2
f_{con}	0.5
f_p	0.87
f_r	0.001
g	0.01
m_{mol}	250 g mol^{-1}
m_{om}	0.10 kg kg^{-1}
k_p	0.0693 d^{-1}
k_{pot}	0
$k_{w,cds}$	0
q_{cds}	0.8 m^3 ha^{-1} d^{-1}
$r_{a,p}$	200 s m^{-1}
$r_{a,pot}$	200 s m^{-1}
$r_{a,r}$	200 s m^{-1}
$r_{a,w,cds}$	200 s m^{-1}
A_i	1 kg ha^{-1}
F	0.2
GAI	1.08
H_a	6 m
$H_{w,cds}$	0.0532 mm
LAI	5
N_{vent}	50 d^{-1}
α	0.07
ε	0.3
θ	0.3
P_{pot}	1 kg/L

System with a permanent water layer on tables

Calculations were made for a simplified version of SEM-P, i.e. a system consisting of plants, pots, roof, greenhouse air, condensation water and a permanent water layer on the tables with a constant temperature in the greenhouse of 20°C. The mass in the water on the tables per surface area of greenhouse (A_{tab}, kg m^{-2}) was simulated by:

$$\frac{dA_{tab}}{dt} = J_{cds} + \left(J_{d,tab} - J_{v,tab}\right) \qquad \text{Eqn 52}$$

$$c_{w,tab} = \frac{A_{tab}}{H_{w,tab}} \qquad \text{Eqn 53}$$

where $c_{w,tab}$ is the concentration in the water on the tables and $H_{w,tab}$ is the volume of water on the tables per surface area of greenhouse (set to 0.0125 m^3 m^{-2}). So it was assumed that the pesticide present in the condensation water is added to the water on the tables and uptake of the pesticide by the pots via the uptake of irrigation water was ignored. Calculations were made for a spray application and parameters as in Table 16 with $c_{w,sol}$ ranging between 1 and 1000 mg/L, P_{sat} ranging between 10^{-6} and 3×10^{-3} Pa, and with K_{om} = 0 or 10 000 L/kg; the simulation period was 1 or 10 d; the compartment thickness was 0.1 mm to be certain of sufficient accuracy. The direct deposition on the tables was 9% in these calculations so at the start of each simulation 9% of the dose was assumed to be present in the water on the tables which is assumed to be representative of the recirculation water.

The gas fluxes for the exchange between the water on the tables and the air were described by:

$$J_{d,tab} = (1 - f_{pot})\ \frac{c_{a,g} - c_{a,tab}}{r_{a,w,tab}} \qquad \text{Eqn 54}$$

$$J_{v,tab} = (1 - f_{pot})\ \frac{c_{a,tab} - c_{a,g}}{r_{a,w,tab}} \qquad \text{Eqn 55}$$

where $J_{d,tab}$ is the mass flux of pesticide (kg m^{-2} d^{-1}) from the air to the water on the tables, $J_{v,tab}$ is the mass flux of pesticide (kg m^{-2} d^{-1}) from the water on the tables to the air, $c_{a,tab}$ is the concentration in the gas phase at the interface between the water and the air (kg m^{-3}), and $r_{a,w,tab}$ is the boundary layer resistance (d m^{-1}) at the water surface set at 200 s/m. The concentration $c_{a,tab}$ was calculated from the concentration in the water on the tables ($c_{w,tab}$ in kg m^{-3}) using Henry's law.

The output considered was the percentage of the dose present in the water on the tables assuming that emission loads are approximately proportional to this percentage.

Results

System with dry table at application time

We consider first a system with K_{om} = 0. Figure 14 shows that the percentage in the water decreases with increasing P_{sat} for $c_{w,sol}$ = 1 or 10 mg/L and that the percentage after 10 d is almost equal to that after 1.2 d after application. This is because there is almost no contribution from the condensation water to this percentage so increasing P_{sat} leads to more volatilisation of the 9% initially deposited onto the dry table. This figure shows that for $c_{w,sol}$ = 1000 mg/L a different pattern: the percentage has a minimum at P_{sat} = 10^{-3} Pa after 1.2 and a maximum at this P_{sat} after 10 days. The increase due to the higher solubility is caused by the increasing contribution of the condensation water to this percentage and there is maximum after 10 days because of the increasing loss by ventilation at higher vapour pressures (32% for P_{sat} = 10^{-3} Pa and 49% loss for P_{sat} = 3×10^{-3} Pa).

Figure 15 shows that increasing the K_{om} to 10 000 L/kg had almost no effect on the results which is at first glance somewhat surprising. This increase led to considerable higher percentages in the pots after 10 d for water solubilities of 1-100 mg/L (e.g. for P_{sat} = 10^{-3} and $c_{w,sol}$ = 10 mg/L there was 1% in the pots for K_{om} = 0 and 21% for K_{om} = 10 000 L/kg). However, differences for a solubility of 1000 mg/L were only comparatively small. The differences between the percentages in the pots become small at higher solubilities because then the flux from the greenhouse air to the pots is controlled by the boundary layer resistance of the air ($r_{a,pot}$) and thus becomes independent of the K_{om} (see Annex 9 for details). In the cases of large differences (e.g. the 1 versus 21%), inspection of the material balance showed that the increase of the percentage in the pots was compensated to a large extend by decreases of ventilation losses and degraded amounts on plants. So the amount of pesticide in the pots then acts on this time scale of 10 d more or less as a sink which competes with the other sinks (although eventually all the pesticide in the pots will volatilise because no degradation in the pots was assumed; see Table 16).

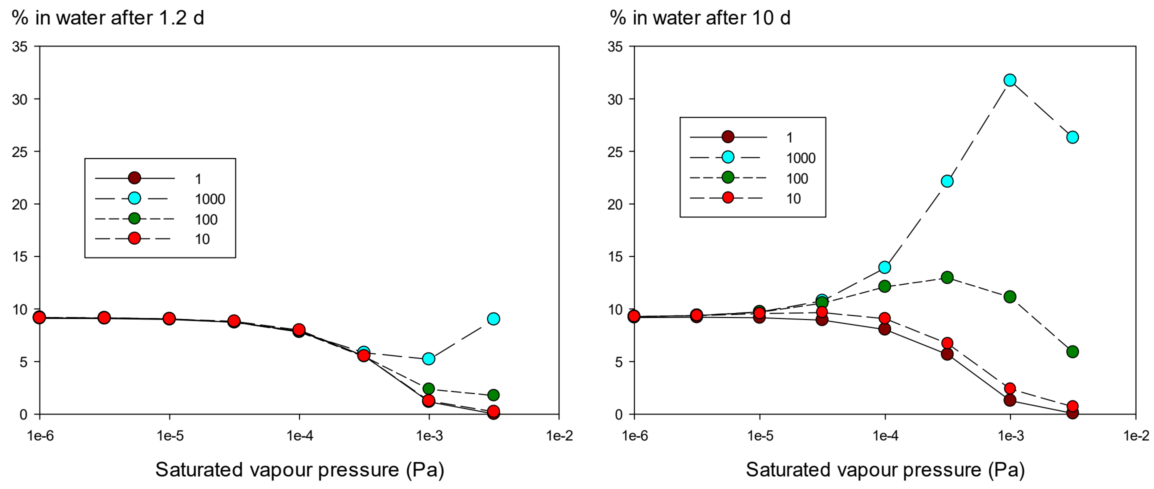


Figure 14 *Effect of saturated vapour pressure on percentage in recirculating water for the SEM-P system with a dry table that is irrigated 1 d after application for* K_{om} *= 0 and water solubilities as indicated in mg/L.*

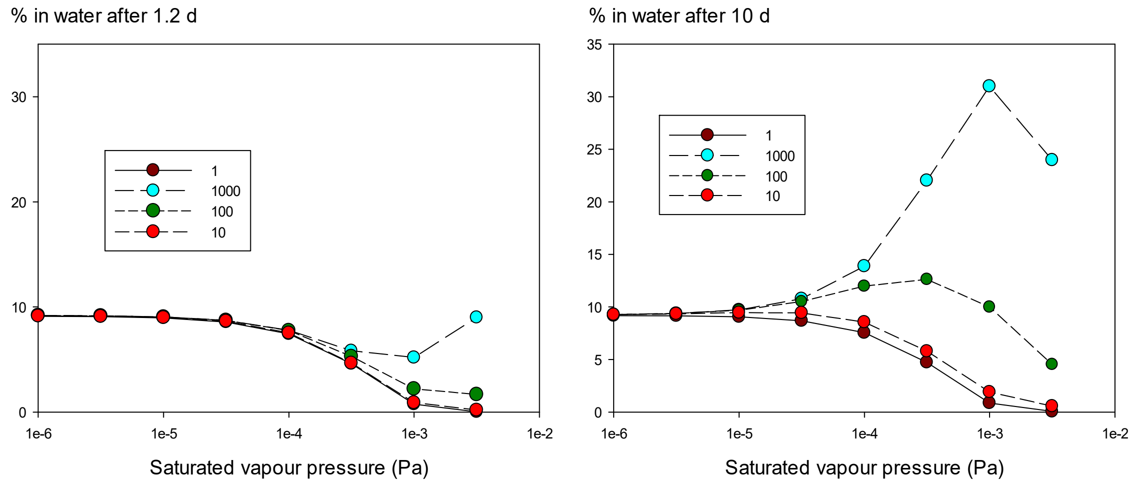


Figure 15 *Effect of saturated vapour pressure on percentage in recirculating water for the SEM-P system with a dry table that is irrigated 1 d after application for* K_{om} *= 10 000 L/kg and water solubilities as indicated in mg/L.*

System with permanent water layer on tables

Figure 16 and Figure 17 show that the percentage in the recirculating water increases with increasing water solubility; this could be expected because increasing the water solubility leads to higher concentrations in the water on the table for a given concentration in the gas phase. The percentage remains almost constant at the initial values of 9% for P_{sat} below 10^{-5} Pa because for non-volatile pesticides the gas fluxes are negligibly small and the pesticide disappears from the system mainly due to degradation at the plant surface. For higher P_{sat} values and $c_{w,sol}$ of at least 10 mg/L the percentage in the water after 1 d increases with increasing P_{sat} and the percentage after 10 d shows an optimum. Inspection of the material balance of the runs showed that the decrease at $P_{sat} = 3\times10^{-3}$ Pa was caused by an increased loss due to ventilation. The percentage decreased with increasing P_{sat} for $c_{w,sol}$ = 1 mg/L because of high ventilation losses.

Comparison of Figure 16 and Figure 17 shows that the effect of the K_{om} on the percentage in the recirculating water was again small. This could be expected for the solubilities above 100 mg/L because then the K_{om} has only a small effect on the percentage in the pots (see for explanation the results of the system with the dry table at application time). Inspection of the material balance for the higher solubilities showed again that higher percentages in the pots for K_{om} = 10 000 L/kg were to a large extent compensated by lower losses due to ventilation and degradation on the plants.

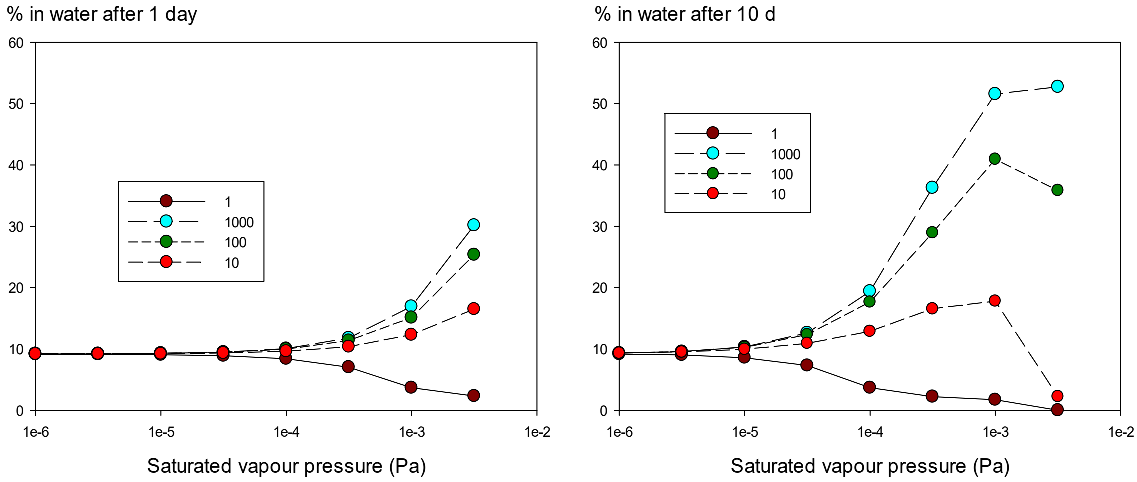


Figure 16 *Effect of saturated vapour pressure on percentage in recirculating water for the SEM-P system with a permanent water layer on the table for* K_{om} *= 0 and water solubilities as indicated in mg/L.*

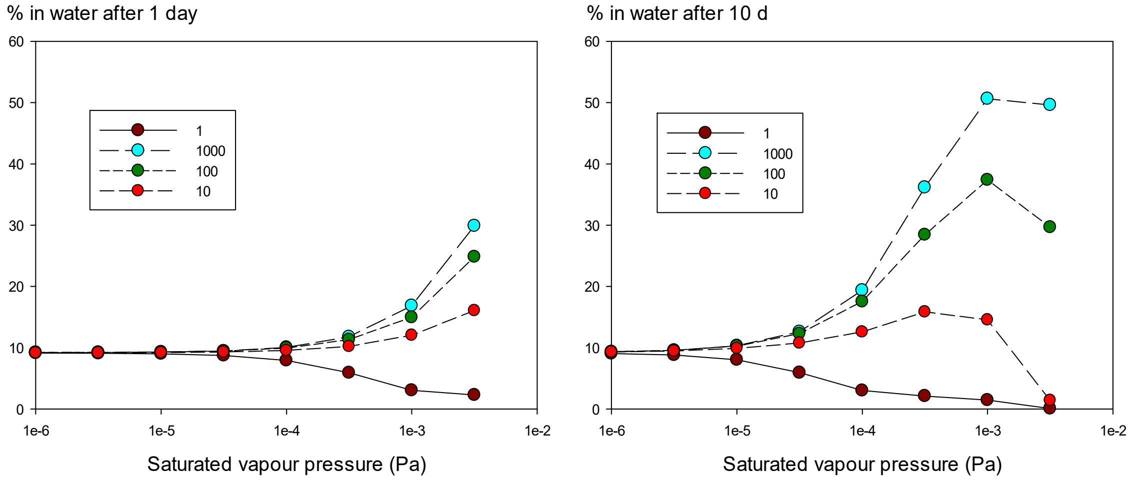


Figure 17 *Effect of saturated vapour pressure on percentage in recirculating water for the SEM-P system with a permanent water layer on the table for* K_{om} *= 10 000 L/kg and water solubilities as indicated in mg/L.*

Discussion and conclusions

It is a priori unknown whether the 'dry-table system' will result in higher or lower emissions than the 'wet-table system': the dry-table system will result in initially lower concentrations because part of the 9% of the dose is volatilised before it is taken up by the water; however, after the irrigation event the percentage of the dose in the water in the dry-table system can only increase (due to the contribution of the condensation water) because no exchange is assumed between the water and the greenhouse air whereas the wet-table system will receive the full 9% of the dose but part of this may also volatilise again from the water leading to a decrease in concentrations. This is confirmed by comparing Figure 14 and Figure 15 with Figure 16 and Figure 17 (note the difference in vertical scales): for water solubilities above 1 mg/L and saturated vapour pressures above 10^{-5} Pa the wet-table system generated higher percentages than the dry-table system and the opposite was true for a water solubility of 1 mg/L and saturated vapour pressures above 10^{-5} Pa. Pesticides with a saturated water pressure above 10^{-5} Pa and a solubility equal to or below 1 mg/L were not in the list of the most important pesticides applied to pot plants compiled by Wipfler et al. (2015). So probably this more realistic description of the water level will lead to lower emission estimates.

Considering the properties of the seven most important pesticides applied to pot plants in Figure 11, we expect that the direct contamination of the water on the tables will be by far the most important source of contamination of the recirculation water for six of the seven: only for the pesticide in the most upper right part, the condensation water may contribute significantly (note that the percentage deposited on the tables has changed into 42% whereas calculation results shown in this annex were still based on 9% deposition on the tables).

Annex 9 Analysis of the penetration depth in pots on tables

It seems worthwhile to get a feeling with respect to the penetration depth of the pesticide in the soil in the pots as we propose a layer of 5 cm thick. Ignoring degradation, Eqn 59 can be rearranged into:

$$\frac{\partial c_{l,pot}}{\partial t} = \frac{D_{dif,g}\, K_H + D_{dif,l}}{\varepsilon K_H + \theta + \rho_{om}\, m_{om}\, K_{om}} \frac{\partial^2 c_{l,pot}}{\partial z^2} \qquad \text{Eqn 56}$$

Thus an ‘effective’ diffusion coefficient D_{eff} can be defined as:

$$D_{eff} = \frac{D_{dif,g}\, K_H + D_{dif,l}}{\varepsilon K_H + \theta + \rho_{om}\, m_{om}\, K_{om}} \qquad \text{Eqn 57}$$

The product $\varepsilon\, K_H$ is always much smaller than θ because K_H is orders of magnitude smaller than 1 for all pesticides except soil fumigants. So this equation indicates that D_{eff} increases with increasing K_H and decreasing K_{om}. Wipfler et al. (2015) selected the most frequently used pesticides in greenhouses. For SEM-P, six pesticides and a plant growth regulator were selected. The K_H ranged from 10^{-14} to 10^{-5} and the K_{om} from 3 to about 18 000 L/kg. Calculated values of D_{eff} ranged from 10^{-5} to 10^{-9} m^2/d.

According to Crank (1975) the analytical solution for a semi-infinite system with an initially zero concentration and a constant concentration at the surface is given by:

$$\frac{c_{l,pot}}{c_{l,0}} = erfc\left(\frac{z}{2\sqrt{D_{eff}\, t}}\right) \qquad \text{Eqn 58}$$

where $c_{l,0}$ is the constant concentration at the surface (kg m^{-3}) and t is time (d). The time available for diffusion in SEM-P is in the order of 10 d because most of the pesticide is deposited on the plants and the default half-life for degradation on the plants is 10 d. Figure 18 indicates that for D_{eff} ranging from 10^{-5} to 10^{-9} m^2/d the penetration is likely to be limited to the top 5 cm.

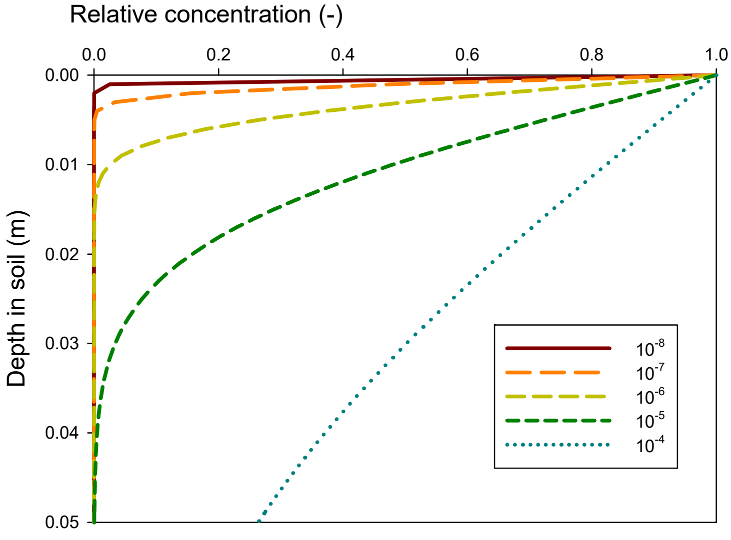


Figure 18 *The relative concentration ($c_{l,pot}/c_{l,0}$) as a function of depth after 10 days for values of D_{eff} as indicated in m^2/d calculated with the analytical solution from Crank (1975).*

The analytical solution from Crank (1975) was compared to the numerical solution in SEM-P for a pesticide with a K_H of 10^{-4} and a K_{om} of 10 L/kg, corresponding with D_{eff} = 7.78 × 10^{-6} m^2/d. Results in Figure 19 show good correspondence between the two solutions.

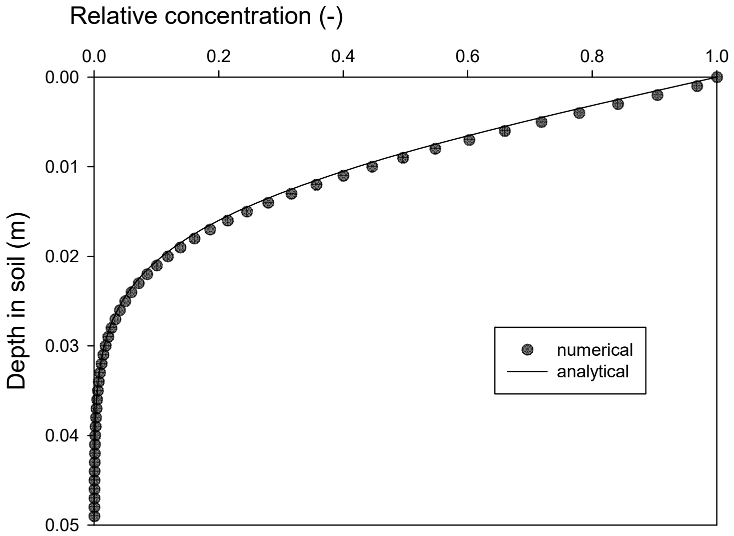


Figure 19 *Comparison between the numerical solution of the concentration in the top 5 cm of the pots after 10 days as calculated with SEM-P with the analytical solution from Crank (1975) for a pesticide with a* K_H *of* 10^{-4} *and a* K_{om} *of 10 L/kg.*

Annex 10 Sensitivity of emission via condensation water to K_{om} assessed with a simplified version of SEM-P

Procedure

Calculations were made for a strongly simplified version of SEM-P, i.e. a system consisting only of plants, pots, roof and condensation water with a constant temperature in the greenhouse of 20°C (so no water layer on the tables or volatilisation from the dry tables). The aim of this was to gain insight of the effect of introducing pots into the system on the emission via the condensation water, keeping in mind that the direct deposition on the tables in the full version of GEM is 41-42% (see Section 4.4.2). We considered the cumulative percentage flown to the clear-water tank as the output that characterises the emissions, so processes in the recirculating water were ignored. Further parameter values are given in Table 16. Calculations were made only for a spray application in view of the small differences to be expected for an LVM-application.

Calculations were made for $c_{w,sol}$ = 1, 10, 100 and 1000 mg/L, P_{sat} = 10^{-6},10^{-5},10^{-4}, 10^{-3} and 10^{-2} Pa and K_{om} = 0 or 10 000 L/kg and a simulation period of 10 d; the thickness of the numerical compartments in the pots was 0.1 mm to be certain of sufficient accuracy.

Effect of pesticide properties on percentage of dose in pots

The percentage left in the pots after these 10 d ranged from 0 to 16% for K_{om} = 0 and from 4-25% for K_{om} = 10 000 L/kg (Figure 20). Increasing the water solubility increased the percentage in the pots for K_{om} = 0: this is understandable because increasing the water solubility leads to increased partitioning into the water in the pots. However, for K_{om} = 10 000 L/kg the percentage increases with increasing the solubility up to 100 mg/L but the percentage for 1000 mg/L is lower than that for 100 mg/L. Comparison between the results for K_{om} = 0 and K_{om} = 10 000 L/kg shows that for solubilities up to 100 mg/L the percentage for 10 000 L/kg is higher than that for 0 (except for low vapour pressures which result all in 4% in the pots, i.e. the initial deposition on the pots). However the solubility of 1000 mg/L resulted in about equal percentages in the pots for 0 and 10 000 L/kg. Additional calculations for a solubility of 100 000 mg/L showed that percentages for 0 and 10 000 L/kg were almost exactly equal. This was at first glance surprising so we considered this in more detail. At these high water solubilities the K_H becomes extremely low (e.g. 10^{-7} for P_{sat} = 10^{-3} and c_{sol} = 1000 mg/L). Under these conditions the concentration in the gas phase at the surface of the pots ($c_{g,pot,sur}$ calculated by Eqn 62) was found to be almost exactly equal to the concentration in the gas phase in the top compartment of the soil. This means that the resistance for diffusion into or out of the pots is controlled by the resistance in the air layer (if there would be no resistance in the air layer, the concentration in the gas phase at the surface of the pots would be equal to that in the greenhouse air). This is understandable because the concentrations in the air are extremely low due to the low K_H so the substance flux from the air to the pots is very slow. So under these circumstances the sorption properties of the pots do not matter anymore (on this time scale of 10 d).

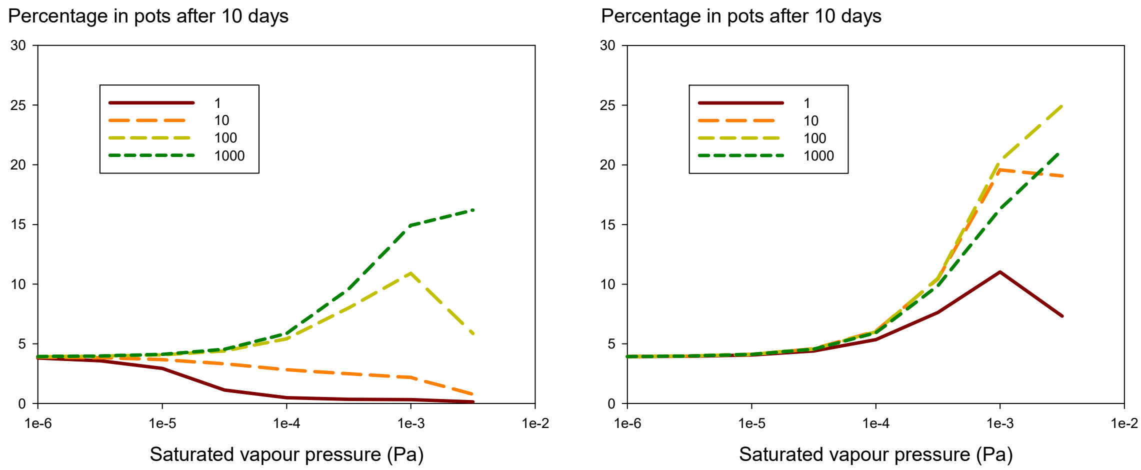


Figure 20 *Percentage of dose in the pots after 10 d as a function of saturated vapour pressure for the SEM-P system consisting of only plants, pots, roof and condensation water for K_{om} = 0 (left) and K_{om} = 10 000 L/kg (right) and water solubilities as indicated in mg/L.*

Effect of pesticide properties on percentage of dose left via the condensation water

In all cases the percentage left via the condensation water increased with increasing $c_{w,sol}$ (Figure 21). This percentage increased initially with increasing P_{sat} but decreased for higher P_{sat} values. This decrease for higher P_{sat} values was the result of an increased loss via ventilation (similar to SEM-P). The effect of increasing the K_{om} from 0 to 10 000 L/kg on the percentage left via the condensation water was surprisingly small (see Figure 21).

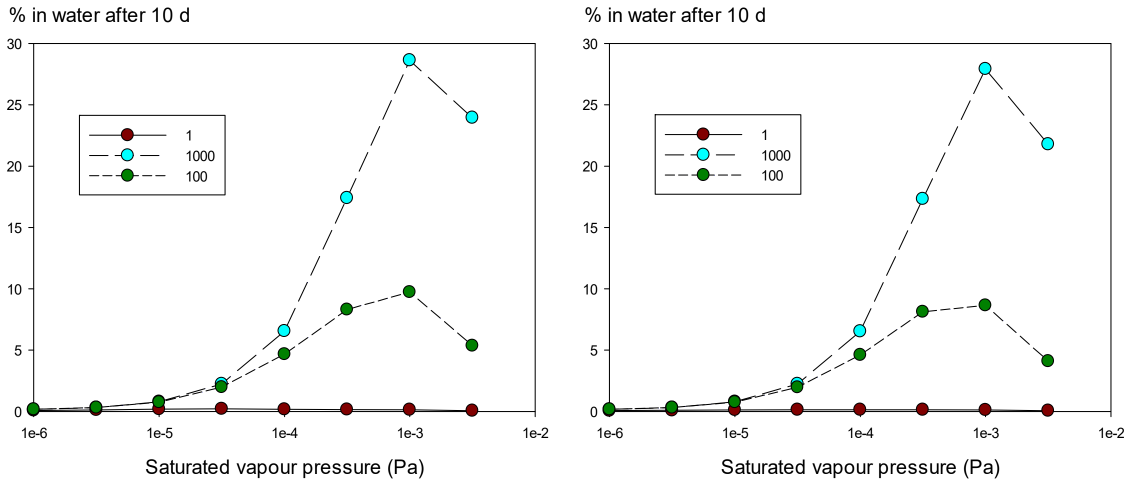


Figure 21 *Effect of saturated vapour pressure on percentage left via condensation water after 10 d for the SEM-P system consisting of only plants, pots, roof and condensation water for K_{om} = 0 (left) and K_{om} = 10 000 L/kg (right) and water solubilities as indicated in mg/L.*

Explanation of small effect of K_{om} on percentage left via condensation water if K_{om} has a large effect on percentage in pots

It will be clear that the effect of K_{om} is small if its effect on the percentage in the pots is small. However, it is not clear why this effect is small if there is a large effect on the percentage in the pots.

So the calculations were made for P_{sat} = 10^{-3} Pa and $c_{w,sol}$ = 10 mg/L, i.e. a relatively volatile pesticide with a moderate solubility that showed a large difference between the percentages in the pots and a small difference between the percentages left via the condensation water for K_{om} = 0 and K_{om} = 10 000 L/kg (2 versus 20% in pots as shown by Figure 20 and 1.3 versus 1.1% left via the condensation water after 10 days, data not shown in Figure 21). Table 17 shows that for this combination of P_{sat} = 10^{-3} Pa and $c_{w,sol}$ = 10 mg/L the percentage left via the condensation water varies only between 1.1

and 1.5% (after 20 days) when the K_{om} is varied between 0 and 100 000 L/kg. It is worthwhile to include also the option of ignoring the diffusion flux into and from the pots (i.e. the 'no pot fluxes' option in the table). The direct deposition on the tables is 9.12% in these calculations and the deposition on the pots is 3.91%. So for the 'no pot fluxes' the percentage in the pots remains constant at 3.91%. For K_{om} = 0, this percentage decreases to 0.08% due to diffusion out of the pots, leading to a slight increased percentage left via condensation water (1.52% versus 1.45%). For the higher K_{om} values the percentages in the pots are after 20 days considerably higher than the initial 3.91%. However, the K_{om} has only a small effect on the percentage left via the condensation water because the increase of the percentage in the pots is almost equal to the sum of the decreases of the percentage ventilated and the percentage transformed on the plants.

The time courses of the percentages in the pots for this pesticide with P_{sat} = 10^{-3} Pa and $c_{w,sol}$ = 10 mg/L (Figure 22) show that for K_{om} = 0 the percentage decreases quickly to about 1% and then remains about constant until 10 days followed by a decrease thereafter. For the higher K_{om} values the percentages increase until about 10 days and decrease slowly thereafter. The calculations of Figure 18 showed that the penetration in soil is deeper for higher D_{eff} values, so deepest for K_{om} = 0. Nevertheless, the release of the amounts in the pots into the air is fastest for K_{om} = 0. Obviously, the K_{om} has a larger effect on the speed of this release than the depth of penetration.

Table 17 *Items of material balance of simplified version of SEM-P (expressed as percentages of the added amount) after 20 days of simulation as a function of the* K_{om} *for a spray application of a substance with* P_{sat} = 10^{-3} *Pa and* $c_{w,sol}$ = *10 mg/L. 'No pot fluxes' means that the flux to and from the pots was set to zero. The percentages do sum up to 91% because 9.12% is assumed to be deposited on the tables. After 20 days, the amounts on the plants and the roof were less than 0.00% (not shown in the table).*

System		In pots (%)	Ventilated (%)	Left via condensation water (%)	Transformed on plants (%)
No pot fluxes		3.91	56.8	1.45	28.7
K_{om} (L/kg)	0	0.08	59.6	1.52	29.7
	100	6.65	55.6	1.43	27.1
	10000	18.88	46.5	1.19	24.3
	100000	21.09	44.6	1.14	24.1

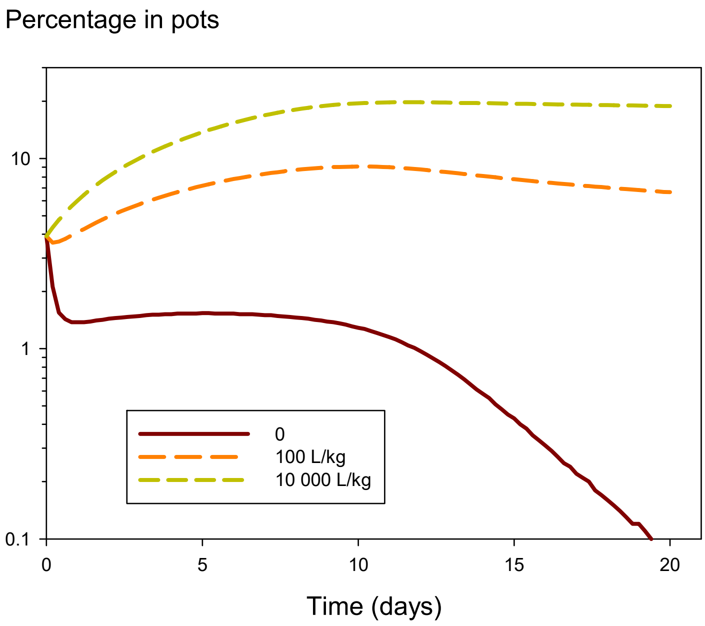


Figure 22 *Percentage in pots as a function of time for three* K_{om} *values as indicated for a substance with* P_{sat} = 10^{-3} *Pa and* $c_{w,sol}$ = *10 mg/L.*

The time courses of the concentration in the greenhouse air (Figure 23, left part) show only a moderate effect of the K_{om} value. Initially, the concentrations are close to 20% of the saturated concentration because the concentration at the plant surface is close to 20% because $F = 0.2$.

The time courses of the concentration in the condensation water (if expressed as percentage of the water solubility, not shown in the figure) were always close to the curves of the concentration in the greenhouse air as shown in left part of Figure 23. This was expected because this substance has a K_H of 10^{-5} (so the time constant for exchange between the air and the water was about 0.1 d). The concentration in the gas phase of the top compartment of the soil (Figure 23, right) follows quite closely the line for that in the greenhouse air for $K_{om} = 0$ (Figure 23, left). For $K_{om} = 100$ L/kg, the concentration in the soil is somewhat lower than in the greenhouse air until about 10 days (leading to the increasing percentage in the pots in Figure 22) and for $K_{om} = 10\ 000$ L/kg the concentration in the soil is considerably lower than in the greenhouse air until about 10 days, leading to the strongly increasing percentage in the pots in Figure 22.

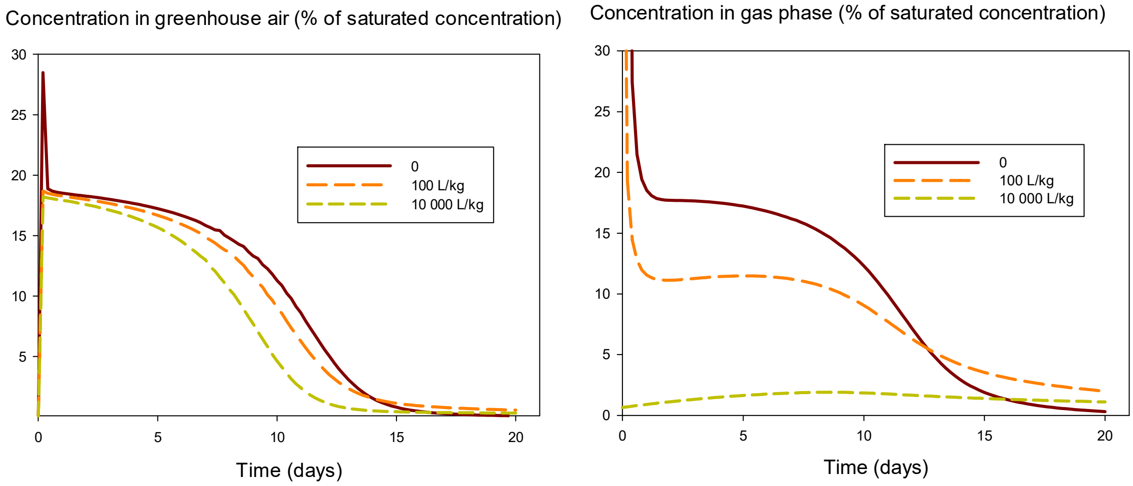


Figure 23 *Concentration of pesticide in greenhouse air (left) and in the gas phase of the top compartment of the soil in the pots (right), both expressed as percentage of the saturated concentration) as a function of time for three* K_{om} *values as indicated for a substance with* $P_{sat} = 10^{-3}$ *Pa and* $c_{w,sol} = 10$ *mg/L.*

Conclusions

The percentage of the dose present in the pots due to exchange between the pot surface and the greenhouse air (so not considering the route via uptake of water by the pots) increases with increasing K_{om} on a time scale of 10 d except for pesticides (i) with solubilities of 1000 mg/L or higher, or (ii) with low saturated vapour pressures. If the solubility is 1000 mg/L or higher, the deposition of pesticide onto the pots is controlled by the resistance for diffusion in the boundary air layer and therefore the K_{om} has almost no effect on the percentage of the dose present in the pots. If the saturated vapour pressure is very low, then the substance flux between the pots and the air is very slow and the percentage in the pots remains at its initial value.

However, the K_{om} has in general only a small effect on the percentage left via condensation water even if the K_{om} has a large effect on the percentage in the pots. The background is that the pots act as a buffer that stores and releases pesticide and an increase of the percentage in the pots is compensated for by approximately equal decreases of the amount lost by ventilation and the amount transformed on the plants.

Wageningen Environmental Research
P.O. Box 47
6700 AA Wageningen
The Netherlands
T +31 (0)317 48 07 00
www.wur.nl/environmental-research

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